

Effect of Reactive Intermediates on the Propagation of Turbulent Premixed Flames

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The most simple version of the Bray and Libby model of turbulent flame propagation has been extended to include a two-step reaction mechanism in which reactants decompose into reactive intermediates which then form products. A transport equation for the joint pdf of intermediate and product concentrations was derived, the pdf parameterized, and transport equations for the parameters obtained. The one-dimensional concentration equations were then solved for the parameters of the pdf and the turbulent kinetic energy. Flame speed and angle are recovered as eigenvalues of the problem. The results show the essential features observed in experiments. The product pdf is composed of peaks at zero and unity product concentration, with a continuous structure representing partially reacted gas. The intermediates pdf has a peak at zero concentration and a broad bell-shaped distribution at nonzero concentration, representing partially reacted gas. The results also show the effect of partitioning of energy release on the flame thickness and speed.

I. Introduction

ONE of the most intriguing aspects of chemically reacting turbulent flows is the mutual interaction of reaction kinetics and fluid dynamics that produces flame behavior. The conservation equations that describe the evolution of flames are, however, inhomogeneous and nonlinear. Thus, practical solution requires simplification of the reaction rate terms and closure assumptions to linearize the equations.

Most workers start their analysis by assuming that the reaction kinetics can be treated as a single-step mechanism in which reactants are converted directly to products at a global rate given by an Arrhenius-type expression. It is well known that even simple fuels are oxidized to final products via quite complex mechanisms, and that reactive intermediate species play an important role in flame behavior.¹⁻⁵ Since we have made measurements of the OH radical in a turbulent flame,⁶ our goal is to develop a model that goes beyond the single-step assumption by including reactive intermediates in the analysis, yet is simple enough to be readily compared with experimental data.

One approach to providing closure that seems more satisfying physically than other schemes is to use probability density functions (pdf's) to provide the statistics of fluctuating parameters. The pdf approach was initiated by Lundgren^{7,8} to study velocity fluctuations in nonreacting turbulent flows, and has more recently been extrapolated to turbulent reacting flows.⁹⁻¹³ Bray and Libby¹⁴⁻¹⁶ introduced the concept of using pdf's to describe the passive scalars temperature or reaction progress variable. They used the pdf concept to analyze turbulent flame propagation in the limit of fast chemistry, intense turbulence, and large turbulent length scale.

We follow the Bray and Libby analysis in its simplest form, except that we include a two-step reaction mechanism and incorporate a joint pdf for intermediates and products. Guirguis et al.⁵ have shown that for methane-air combustion one may group species into pools of reactant, intermediates, and products which are approximately tied to one another

kinetically. The reaction mechanism is thus modeled as a two-step process where the reactants R form a pool of intermediate radicals I which then react to form products P . A transport equation for the joint pdf of I and P is introduced, together with the basic governing equations of mass, momentum, and kinetic energy of turbulence. The pdf is then parameterized and transport equations for each of the pdf parameters derived.

In the following, the conservation equations for mass, momentum, turbulent kinetic energy, and joint pdf are outlined. The analysis and method of solution are next described. The calculated results are presented and discussed. Finally, the study is summarized and conclusions drawn.

II. Theoretical Model

The flow considered is an oblique infinite plane flame propagating into a grid-produced turbulent flow of premixed methane-air. Figure 1 shows the coordinate system adopted for the analysis.

The reaction mechanism is modeled in two steps of the form:



We assume that the reactants, intermediates, and products may be treated as ideal gases. We also assume that the specific heats of each component are constant, the flow is adiabatic, the Mach number is low, pressure fluctuations are small, and the Lewis number is unity. These assumptions lead to a simple relationship between temperature and the mass fractions, allow neglect of pressure changes and viscous dissipation, and simplify the analysis of diffusion.

A. Conservation Equations

The one-dimensional Favre-averaged conservation equations for mass, momentum, and turbulent kinetic energy were given by Bray and Libby in Ref. 14, in which they assumed that the mean streamline undergoes negligible deflection as it crosses the reaction zone. We adopt the undeflected mean streamline assumption, even though Libby and Bray have since developed a more complete model,¹⁷ because it relaxes the dependence of the flow parameters on the y direction, simplifying the governing equations. The consequence of the assumption is that the two velocity components may be simply

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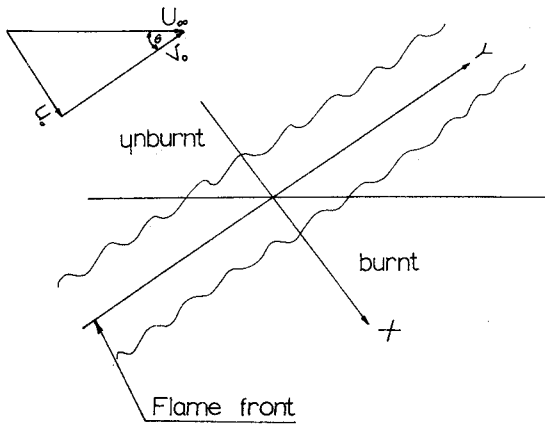


Fig. 1 Coordinate system.

related as

$$\tilde{u} = \tilde{v} \tan \theta \quad (3)$$

where \tilde{u} and \tilde{v} are the Favre-averaged velocity components in the x and y directions, respectively, and θ is the flame angle.

Following the Bray and Libby model¹⁴ the one-dimensional conservation equations become:

Conservation of mass:

$$\frac{d}{dx}(\rho \tilde{u}) = 0 \quad (4)$$

Conservation of x momentum:

$$\frac{d}{dx}(\bar{\rho} \tilde{u}^2 + \overline{\rho u''^2}) = \frac{d\bar{p}}{dx} \quad (5)$$

Conservation of y momentum:

$$\frac{d}{dx}(\bar{\rho} \tilde{u} \tilde{v} + \overline{\rho u'' v''}) = 0 \quad (6)$$

Conservation of kinetic energy of turbulence:

$$\frac{d}{dx}(\rho \tilde{u} \tilde{q} + \overline{\rho u'' q''}) = -\overline{\rho u''^2} \frac{d\tilde{u}}{dx} - \overline{\rho u'' v''} \frac{d\tilde{v}}{dx} \quad (7)$$

where ρ is the density, p the static pressure, and q the kinetic energy of turbulence. The turbulence dissipation and pressure diffusion terms in the turbulent kinetic energy equation have been neglected based on the order of magnitude analysis of Bray and Libby.^{14,18}

Introducing the parameters r , i , and c to describe the mass fraction of reactants, intermediate radicals, and products, respectively, a mass balance would imply that

$$r + i + c = 1 \quad (8)$$

The thermal energy equation under these conditions is

$$H = H_0 + iH_1 + cH_2 \quad (9)$$

where H_1 and H_2 are the heats of reaction associated with the chemical reactions (1) and (2), respectively, and H_0 is the stagnation enthalpy.

The transport equation of the joint pdf of intermediates and products following the previous assumptions is

$$\begin{aligned} \frac{\partial}{\partial t}(\bar{\rho} \tilde{P}) + \frac{\partial}{\partial x}(\bar{\rho} \tilde{u} \tilde{P} + \overline{\rho u'' \kappa}) + \frac{\partial}{\partial i}(\bar{\rho} S(i) \tilde{P}) \\ + \frac{\partial}{\partial c}(\bar{\rho} S(c) \tilde{P}) = \tilde{E} \end{aligned} \quad (10)$$

where $S(m)$ is the chemical source term of species m , \tilde{P} the joint pdf, and \tilde{E} the diffusion of the pdf in probability space.

Finally, the thermodynamic equation of state is

$$\bar{p} = \rho RT \quad (11)$$

where \bar{p} is the pressure and T the temperature.

B. Closure Modeling

The conservation equations require closure of two types of terms. In the momentum, turbulent kinetic energy, and pdf equations there are turbulent diffusion terms which must be evaluated. Although there are more advanced methods available, we follow Bray and Libby¹⁴ in adopting an eddy diffusivity model for simplicity. In the pdf transport equation the diffusion in pdf space term must be evaluated. For simplicity we model this term with a modified form of Curl's coalescence dispersion model.

The turbulent diffusion terms in Eqs. (5-7) and (10) thus become:

$$\overline{\rho u'' g''} = -\nu_T \bar{\rho} \frac{\partial \tilde{g}}{\partial x} \quad (12)$$

where g is a dummy variable that represents the v component of velocity, the turbulent kinetic energy, or the pdf. The turbulent kinematic eddy viscosity ν_T is described by a conventional Prandtl-Kolmogorov model,

$$\nu_T = a \tilde{q}^{1/2} \ell \quad (13)$$

where a is a constant and ℓ is a characteristic length scale of large eddies.

The fraction of the turbulent kinetic energy associated with the term $\rho u'' u''$ may be modeled as a percentage of the kinetic energy, such that

$$\overline{\rho u'' u''} = \epsilon \bar{\rho} \tilde{q} \quad (14)$$

where $0 < \epsilon < 1$.

Curl's coalescence dispersion model implies that whenever two blobs of gases with different concentrations, or temperatures, are brought together by molecular or turbulent mixing, they produce two new lumps with the average concentration and temperature of the original blobs. Curl¹⁹ originally formulated the model for droplet interactions in two-phase chemical reactors. Pratt²⁰ and Pope²¹ extended it to gases and applied it to the diffusion of the pdf in probability space. We thus model the mixing of the pdf in the probability space as:

$$\tilde{E} = \omega \left\{ 4 \iint \tilde{P}(i+i', c+c') \tilde{P}(i-i', c-c') di dc - \tilde{P}(i, c) \right\} \quad (15)$$

where ω is a characteristic frequency of energy-containing motion, taken to be equal to $q^{1/2}/\ell$.

The model is valid if the time scales for molecular and turbulent mixing are short compared to the characteristic time scales of the flow.^{6,22} We use the model for simplicity despite its disadvantages.²³ Janieka et al.²⁴⁻²⁶ have suggested a generalization to avoid the deficiencies of the original model; however, they require adjustment of a constant to fit the rate of decay of the variance, which further complicates the governing equations and lacks experimental verification.

C. Final Form of the Equations

Using the closure models (12-15) and the initial upstream conditions, one can introduce the following nondimensional parameters:

Length scale

$$\eta = x \tilde{u}_0 / (\tilde{q}_0^{1/2} a \ell_0) \quad (16)$$

Time scale

$$t^* = \bar{u}_0^2 / (\bar{q}_0^2 a \ell_0) \quad (17)$$

Turbulence length scale

$$L = \ell / \ell_0 \quad (18)$$

Turbulence kinetic energy

$$Q = \bar{q} / \bar{q}_0 \quad (19)$$

Flame speed

$$V = \bar{u}_0^2 / \bar{q}_0 \quad (20)$$

The subscript zero indicates the value on the cold side of the flame.

Introducing τ_1 and τ_2 to represent the nondimensional heat of reaction, such that

$$\tau_j = H_j / H_0 \quad (21)$$

the final form of Eqs. (4), (9), and (11) will be

$$\frac{\bar{u}}{\bar{u}_0} = \frac{\rho_0}{\bar{\rho}} = \frac{\bar{T}}{\bar{T}_0} = 1 + \tau_1 \bar{i} + \tau_2 \bar{c} \quad (22)$$

The turbulent kinetic energy equation will become

$$\begin{aligned} \frac{dQ}{d\eta} - \frac{d}{d\eta} \left[\frac{\bar{\rho}}{\rho_0} Q^{\frac{1}{2}} L \frac{dQ}{d\eta} \right] \\ = - \left[\epsilon Q \frac{\bar{\rho}}{\rho_0} - \left(\frac{V}{\tan^2 \theta} \right) \left(\frac{\rho_0}{\bar{\rho}} - 1 \right) \right] \frac{d}{dx} \frac{\bar{u}}{\bar{u}_0} \end{aligned} \quad (23)$$

and the pdf transport equation will be

$$\begin{aligned} \frac{\bar{\rho}}{\rho_0} \frac{\partial \bar{P}}{\partial t} + \frac{\partial \bar{P}}{\partial \eta} - \frac{\partial}{\partial \eta} \left[\frac{\bar{\rho}}{\rho_0} Q^{\frac{1}{2}} L \frac{\partial \bar{P}}{\partial \eta} \right] + \frac{\bar{\rho}}{\rho_0} \frac{\partial}{\partial i} [S(i) \bar{P}] \\ + \left(\frac{\bar{\rho}}{\rho_0} \right) \frac{\partial}{\partial c} [S(c) \bar{P}] = \left(\frac{\bar{\rho}}{\rho_0} \right) \tau_j \bar{E} \end{aligned} \quad (24)$$

where the averaged quantities \bar{i} and \bar{c} are obtained by integration

$$\bar{i}(\eta, t) = \int \int i \bar{P}(i, c, \eta, t) di dc \quad (25)$$

and

$$\bar{c}(\delta, t) = \int \int c \bar{P}(i, c, \eta, t) di dc \quad (26)$$

It should be noted that we have not introduced an equation to calculate L , the turbulent length scale. Following Bray and Libby we assume that the turbulent Reynolds number, $\bar{q}_0^2 \ell / \nu_T$, is constant, or $\bar{Q}L = 1$. Therefore Eqs. (23) and (24) will become

$$\begin{aligned} \frac{dQ}{d\eta} - \frac{d}{d\eta} \left[\frac{\bar{\rho}}{\rho_0} \frac{dQ}{d\eta} \right] \\ = - \left[\epsilon Q \frac{\bar{\rho}}{\rho_0} - \left(\frac{v}{\tan^2 \theta} \right) \left(\frac{\bar{\rho}}{\rho_0} - 1 \right) \right] \frac{d}{dx} \left(\frac{\bar{u}}{\bar{u}_0} \right) \end{aligned} \quad (27)$$

and

$$\begin{aligned} \frac{\bar{\rho}}{\rho_0} \frac{\partial \bar{P}}{\partial t} + \frac{\partial \bar{P}}{\partial \eta} - \frac{\partial}{\partial \eta} \left[\frac{\bar{\rho}}{\rho_0} \frac{\partial \bar{P}}{\partial \eta} \right] \\ + \frac{\bar{\rho}}{\rho_0} \left[\frac{\partial}{\partial i} (S(i) \bar{P}) + \frac{\partial}{\partial c} (S(c) \bar{P}) \right] = \frac{\bar{\rho}}{\rho_0} \bar{E} \end{aligned} \quad (28)$$

Equations (22) and (25-28) are a complete set that describes the evolution of the turbulent kinetic energy, the pdf, and the density and velocity. The flame speed V and angle θ are eigenvalues of the solution.

D. Parameterization of the pdf

The solution of the pdf transport equation is hampered by the fact that it is an integrodifferential equation. Thus, one would like to simplify as much as possible. One approach toward simplification is to parameterize the pdf and then derive differential transport equations for the parameters. This is the approach taken by Bray and Libby¹⁴ for the pdf of reaction progress variable.

Parameterization is supported in our analysis by data that were taken of OH number density pdf's in a laboratory scale burner.²⁷ The experimental pdf's consist of a spike at zero concentration and a continuous bell-shaped structure at non-zero concentrations. The continuous structure has zero amplitude on the cold side of the flame. Within the flame it exhibits a broad distribution indicating peak concentrations in excess of equilibrium values. On the hot side of the flame the continuous distribution is quite narrow and peaked at the equilibrium concentration.

We have thus chosen to simulate the zero-concentration spike by a delta function and a separate function for the continuous structure. Ideally, one would like to use a two-parameter function for the continuous structure but, for simplicity in the present analysis we have chosen a gamma function. The peak of the gamma function increases with its variance, so that it should display similar behavior to that observed experimentally. The parameterized form of the pdf is then

$$\begin{aligned} \bar{P}(i, c, \eta) = \alpha(\eta) \delta(i) \delta(c) \\ + \beta(\eta) \delta(i^* - i) \delta(c^* - c) + \Gamma(i, \eta) \end{aligned} \quad (29)$$

where α and β are area coefficients, calculated from the pdf transport equation [24], i^* and c^* are the equilibrium concentration of intermediates and products, respectively, $\Gamma(i, \eta)$ is the gamma distribution function of species i at location η , and δ is the Dirac delta function. The gamma function is defined as

$$\Gamma(i, \eta) = i^{\mu-1} e^{-i} \quad (30)$$

where μ is the mean²⁸ of the distribution. μ is a function of position η .

By substituting the parameterized form of the pdf, Eq. (29), into the pdf transport equation, defining a reduced coordinate as

$$\xi = \int (1 + \tau_1 \bar{i} + \tau_2 \bar{c})^{-1} d\eta$$

and equating the coefficients of the delta functions to zero, one obtains a set of transport equations for the pdf parameters. These are

$$\frac{d}{d\xi} \left[\frac{1}{(1 + \tau_1 \bar{i} + \tau_2 \bar{c})^2} \right] \frac{d\alpha}{d\xi} - \frac{d\alpha}{d\xi} + \alpha^2 - \alpha = 0 \quad (31)$$

and

$$\frac{d}{d\xi} \left[\frac{1}{(1 + \tau_1 \bar{i} + \tau_2 \bar{c})^2} \right] \frac{d\beta}{d\xi} - \frac{d\beta}{d\xi} + \beta^2 - \beta = 0 \quad (32)$$

where μ is calculated from the normalization condition on the pdf

$$1 = \alpha + \beta + c^* \int f(i, \xi) di \quad (33)$$

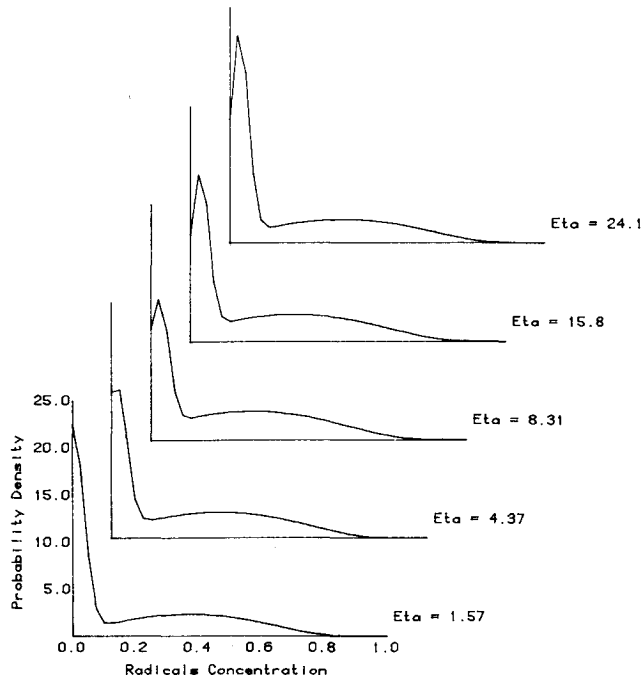


Fig. 2 Products' pdf's.

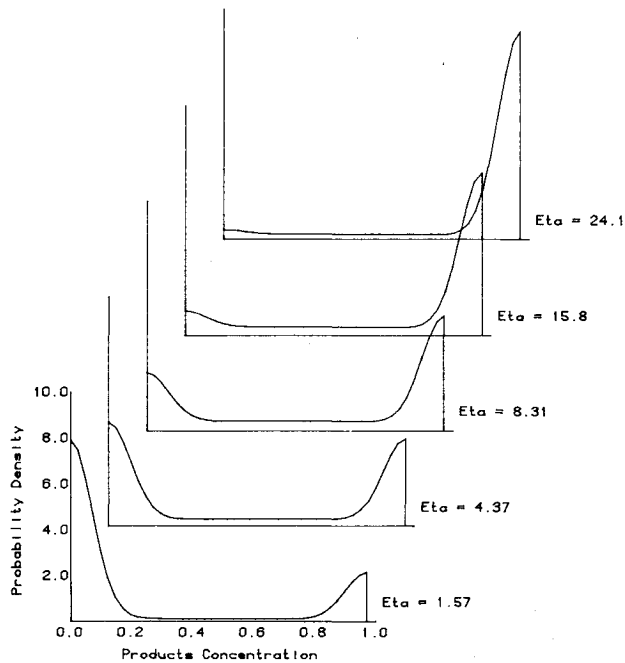


Fig. 3 Intermediates pdf's.

The turbulence kinetic energy equation, using the reduced coordinate ξ , becomes

$$\frac{d}{d\xi} \left[\frac{1}{(1 + \tau_1 \tilde{i} + \tau_2 \tilde{c})^2} \right] \frac{dQ}{d\xi} - \frac{dQ}{d\xi} = - \left[\epsilon Q \left(\frac{\bar{\rho}}{\rho_0} \right) - \left(\frac{V}{\tan^2 \theta} \right) \left(\frac{\rho_0}{\bar{\rho}} - 1 \right) \right] \frac{d}{d\xi} \left(\frac{\rho_0}{\bar{\rho}} \right) \quad (34)$$

where

$$\tilde{i}(\xi) = \int \int i \tilde{P}(i, c, \xi) di dc \quad (35)$$

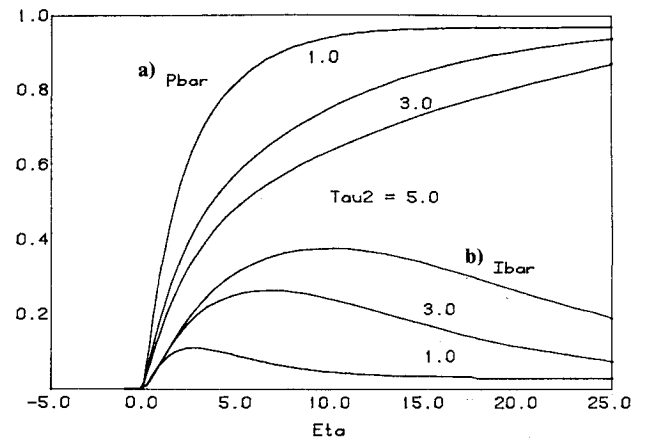


Fig. 4 (a) Average of product concentrations. (b) Average of radical concentrations.

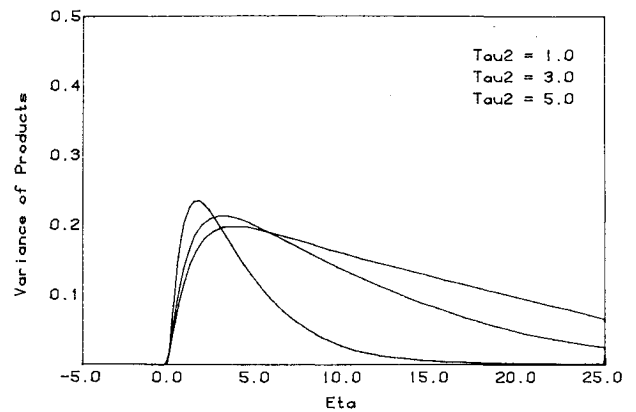


Fig. 5a Variance of product concentrations.

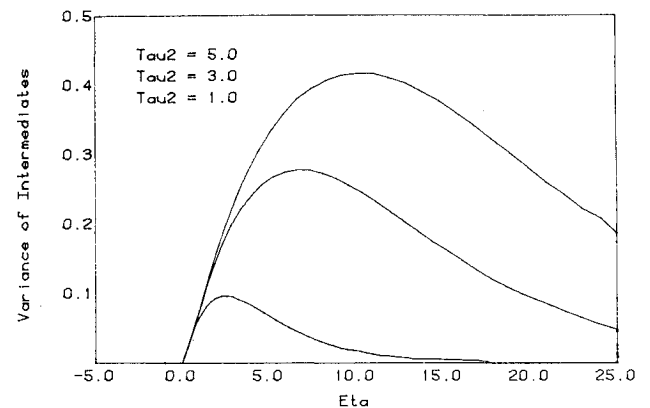


Fig. 5b Variance of radical concentrations.

and

$$\tilde{c}(\xi) = \int \int c \tilde{P}(i, c, \xi) di dc \quad (36)$$

Equations (31-38) form a complete set of governing equations that describe the flowfield. The flame angle θ and speed V are eigenvalues of the solution under the prescribed boundary conditions.

E. Boundary Conditions and Solution

The cold and hot boundary conditions are obtained by asymptotically expanding Eqs. (31-34) near $\xi = \pm \infty$, respec-

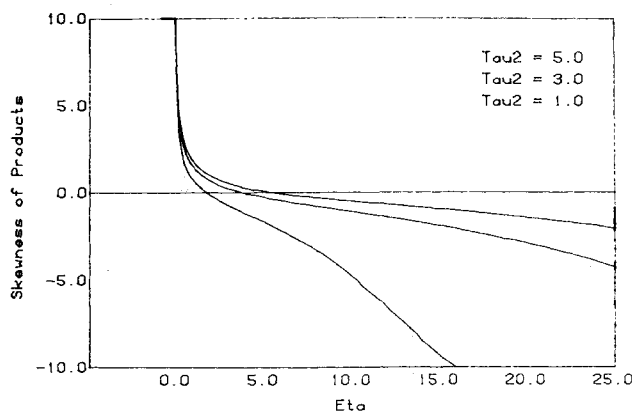


Fig. 6a Skewness of product concentrations.

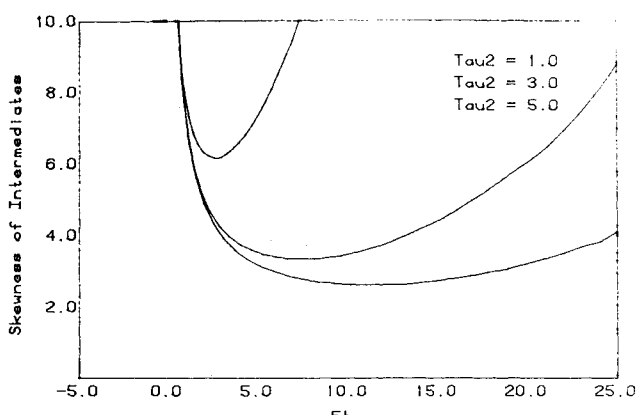


Fig. 6b Skewness of radical concentrations.

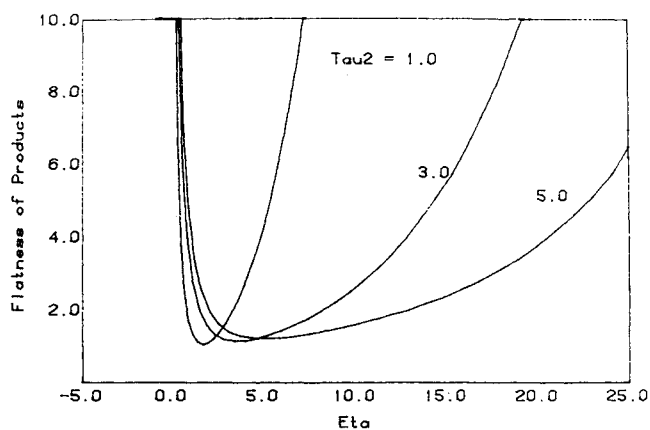


Fig. 7a Flatness of product concentrations.

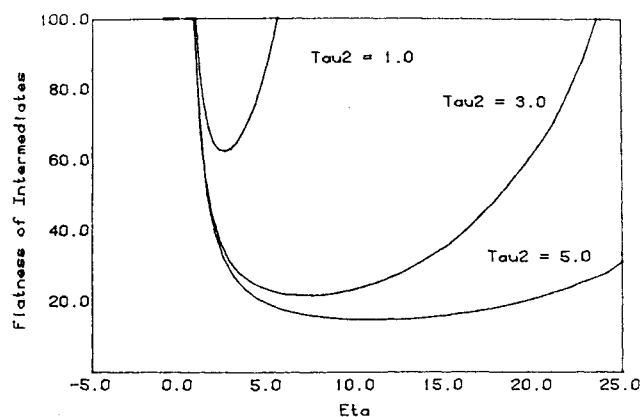


Fig. 7b Flatness of radical concentrations.

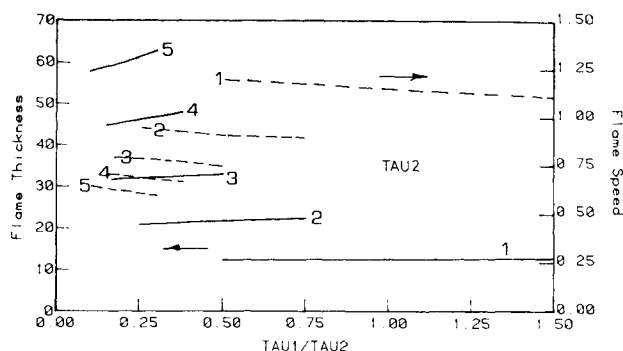


Fig. 8 Flame thickness and speed parameters.

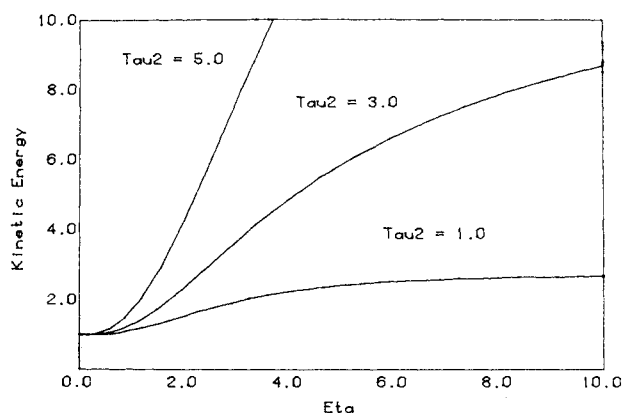


Fig. 9 Kinetic energy of turbulence.

tively. Therefore the cold boundary is represented as

$$g(\xi) = g(0)e^{\xi} \quad \xi \leq 0 \quad (37)$$

where g is a dummy variable that represents α , β , Q , \tilde{c} , and \tilde{i} . In our analysis, we used $\tilde{c}(0) = 0.02$, $\tilde{i}(0) = 0.01$, $\alpha(0) = 0.98$, and $\beta(0) = 0.02$. These values are recommended in Ref. 14.

At the hot side of the flame, the radicals are assumed to reach their equilibrium value, which is calculated using the NASA equilibrium code.²⁹ The equilibrium value of the products is calculated from the normalization condition.

$$I = i^* + c^* \quad (38)$$

Equations (31-36) are solved by dividing the field into cold and hot regions, such that $-\infty < \xi \leq 0$ and $0 \leq \xi < \infty$, respectively. Integration over the two regions is done independently using the boundary conditions discussed above. The flame angle and speed are obtained by matching the two solutions at the point $\xi = 0$.

III. Results

We have calculated the pdf parameters, flame thickness, and speed and turbulent kinetic energy for a variety of values of τ_1 and τ_2 .

Figures 2 and 3 show typical pdf's of product and intermediate radical concentration, respectively, at different flame locations for $\tau_1 = 1.5$ and $\tau_2 = 5.0$. (The calculated pdf's have been convolved with 10% noise, as might typically be seen in an experimental measurement.)

Figure 4 shows the average of the product and radical concentrations for different values of τ_2 . Likewise, Fig. 5 shows the variance, Fig. 6 the skewness, and Fig. 7 the flatness of the product and intermediate concentrations, respectively.

Figure 8 shows the effect of heat release on the 1-99% flame thickness and the flame speed for different values of τ_1 and τ_2 . Figure 9 shows profiles of the turbulent kinetic energy for different values of τ_2 .

IV. Discussion

The calculated pdf's are consistent in appearance with those seen experimentally.²⁷ The product pdf's display two peaks, one at zero concentration and the other at the hot side equilibrium concentration, $c \sim 1$, with an intermediate structure representing partially reacted gas. On the cold side of the flame most of the gas is unreacted and thus one sees a strong zero peak. Within the flame one sees cold, reacting, and reacted gas. This is reflected in the pdf by the appearance of two strong peaks and a fairly high level of intermediate density. On the hot side of the flame the gas consists almost entirely of products; thus one sees a strong peak at $c \sim 1$.

The intermediates pdf also displays two peaks, except that the peak away from zero concentration shifts as one traverses across the flame. On the cold side there is almost all cold reactants and no intermediates. Within the flame there are large quantities of intermediates belonging to parcels of gas at various stages of reaction. Thus one sees a larger variance of the continuous structure. On the hot side of the flame the intermediates present are almost all at equilibrium with the products; thus the variance of the continuous structure is reduced.

One may see the above effects more clearly by examining the parameters of the pdf and its moments directly as shown in Figs. 4-7.

The values of flame thickness and speed are a function of the partitioning of heat release between intermediates and products, as shown in Fig. 8. For a fixed value of total heat release, increasing τ_1 causes the flame to thicken and the flame speed to decrease correspondingly. At small τ_2 the effect of τ_1 is less because of the asymptotic approach of the flame thickness to the turbulent length scale.

V. Summary and Conclusions

We have extended the most simple version of the Bray and Libby model of turbulent flame propagation to include a two-step reaction mechanism in which reactants decompose into reactive intermediates which then form products. A transport equation for the joint pdf of intermediate and product concentrations was derived, the pdf parameterized, and transport equations for the parameters obtained. The one-dimensional concentration equations were then solved for the parameters of the pdf and the turbulent kinetic energy. Flame speed and angle are recovered as eigenvalues of the problem.

The results show the essential features observed in experiments. The product pdf is composed of peaks at zero and unity product concentration with a continuous structure representing partially reacted gas. The intermediates pdf has a peak at zero concentration and a broad bell-shaped distribution at nonzero concentration representing partially reacted gas.

The results also show the effect of partitioning of energy release on the flame thickness and speed.

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