

THE STOCHASTIC FLAMELET MODEL OF TURBULENT PREMIXED COMBUSTION

S. B. POPE

*Sibley School of Mechanical & Aerospace Engineering
Cornell University, Ithaca, NY 14853*

AND

W. K. CHENG

*Mechanical Engineering Department
Massachusetts Institute of Technology
Cambridge, MA 02139*

A new stochastic model is presented and used to calculate the properties of turbulent premixed flames in the flame-sheet regime. The flame sheet is represented statistically by infinitesimal flamelets, each characterized by its position, its unit normal vector, and its (infinitesimal) area. The evolution of the position and normal are completely determined by the fluid velocity and its spatial derivatives following the flamelet, which are modeled by stochastic processes. The flamelet area changes by stretching caused by velocity gradients, by the propagation of cusps, and because of curvature. An additional model is developed to account for the latter two mechanisms.

The Stochastic Flamelet Model is used in conjunction with the joint pdf approach to make calculations of non-stationary, statistically plane turbulent premixed flames. These calculations demonstrate the practicality of the method and illustrate its attributes. Because it contains a natural and comprehensive statistical description of the flame sheet, the model allows the essential physical processes to be incorporated in a straightforward manner.

Introduction

Both in spark ignition engines and in laboratory flames, turbulent premixed combustion most often occurs in the flame-sheet regime.¹⁻³ A thin flame sheet (thinner than the Kolmogorov scale) forms a surface^{4,5}—possibly highly corrugated—that separates reactants from products (see Fig. 1). This flame surface is convected, bent and strained by the turbulence⁶ and propagates (relative to the reactants ahead) at a speed that can depend on the local conditions.

A wide variety of modeling approaches has been applied to turbulent premixed flames in the flame-sheet regime. Some (e.g. Refs. 7-9) aim at calculating global quantities—turbulent flame speed, overall mass-burning rate, etc.—while others (e.g., Refs. 10-14) are more comprehensive in that they attempt to describe the temporal and spatial variations of statistics through the flame. Both the Bray-Moss-Libby model^{10,11} and the pdf method¹²⁻¹⁴ (which are in the latter category) have been successful in accounting for some of the experimental observations related to counter-gradient diffusion and flame-generated turbulence.^{11,14} But both models

have shortcomings in determining the local burning rate. In the Bray-Moss-Libby model the local burning rate is not determined at all,¹¹ and so the turbulent flame speed is required as an input to the calculation rather than emerging as a calculated result. In the pdf method the local burning rate is calculated, but not in an entirely satisfactory manner: the burning rate is (implicitly) assumed to be inversely proportional to the turbulent time scale,^{12,15} and the incorporation of the influence of the laminar flame speed is ad hoc.¹³

The Stochastic Flamelet Model, presented here, provides a method for determining the local burning rate. It does so by explicitly representing the flame sheet and the processes that affect its evolution. The numerical implementation of the model is a Monte Carlo method in which the flame sheet is represented by large numbers of flame elements, or flamelets. Each flamelet has a position, an orientation and an (infinitesimal) area, which evolve according to stochastic models.

The Stochastic Flamelet Model is used in conjunction with the pdf method,¹⁵ there being a two-way coupling between the two methods. A modeled equation is solved for the joint pdf of velocity,

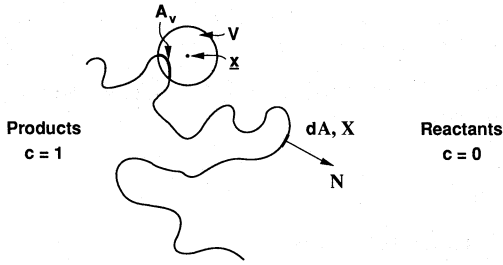


FIG. 1. Sketch of a flame sheet.

dissipation and reaction progress variable, the local mean reaction rate being supplied by the flamelet model. The pdf method determines the mean fields—velocity, progress variable, etc.—required by the flamelet model.

The model is described in the next section. Calculations have been performed for the idealized case of an initially plane flame sheet in constant-density, stationary, isotropic turbulence. These calculations, reported in the third section, prove the practicality of the model and illustrate the influence of the laminar flame speed. Conclusions are drawn in the final section.

The Stochastic Flamelet Model

An infinitesimal flame element—or flamelet—has position $X(t)$, area $dA(t)$, and unit normal $N(t)$ (pointing into the reactants). By definition,⁶ as it evolves, the flamelet remains part of the flame sheet by its position changing according to the equation

$$\dot{X}(t) = U(t) + wN(t). \quad (1)$$

Here $U(t)$ is the fluid velocity just ahead of the flame, and w is the local propagation speed of the flame-sheet relative to the reactants. In the present work we take w to be a constant—the laminar flame speed—but there is no difficulty in allowing for a dependence on the local strain rate.

In the variable-density case, the Eulerian velocity $u(x,t)$ is discontinuous at the flame sheet.⁵ Hence, since $U(t)$ and w are defined with respect to the reactants, we have

$$U(t) = \lim_{y \rightarrow 0} u(X(t) + y|N(t), t). \quad (2)$$

In the constant-density case considered here $u(x,t)$ is continuous, and Eq. (2) reduces to $U(t) = u(X[t], t)$.

The initial condition for Eq. (1) is of great importance. Let S_o denote the flame surface at the initial time t_o . Then the initial flamelet position $X_o = X(t_o)$ is a random variable uniformly distributed

on S_o . Let A_o be the expected[†] initial surface area, and let dA_o be the initial (infinitesimal) area of the flamelet (i.e. $dA(t_o) = dA_o$). We define

$$A(t) \equiv dA(t)/dA_o, \quad (3)$$

to be the area amplification of the flamelet.

From these definitions and a knowledge of the flamelet properties, much useful information can be obtained.⁶ The total expected surface area is

$$A_s(t) = A_o \langle A(t) \rangle, \quad (4)$$

and, most importantly, the expected surface-to-volume ratio is

$$\Sigma(x,t) = A_o \langle A(t) \delta(x - X(t)) \rangle. \quad (5)$$

The importance of the surface-to-volume ratio stems from the following expression for the local expected burning rate $\omega(x,t)$ (volume burned per unit volume per unit time):

$$\omega(x,t) = w \Sigma(x,t). \quad (6)$$

Referring to Fig. 1, this formula can be understood by considering the volume V centered on the point x . On a given realization let $A_v(t)$ be the area of the surface within V at time t . ($A_v(t)$ may well be zero.) In the infinitesimal time interval dt , the volume of fluid burned by the propagating surface within V is $wA_v dt$. Hence the volume-averaging burning rate is wA_v/V . Equation (6) is then obtained as

$$\begin{aligned} \omega(x,t) &= \lim_{v \rightarrow 0} \langle wA_v/V \rangle \\ &= w \Sigma(x,t). \end{aligned}$$

In addition to the equation for $X(t)$ (Eq. 1), evolution equations for $N(t)$ and $A(t)$ can be derived from first principles.⁶ They are:

$$\dot{N}_i = N_i N_j N_k U_{j,k} - N_j U_{j,i}, \quad (7)$$

and

$$\dot{A} = -AN_i N_j U_{ij} - \dot{A}_R, \quad (8)$$

where U_{ij} denotes the velocity derivative $\partial u_i / \partial x_j$ in the reactants just ahead of the flamelet. The initial condition $N(t_o)$ is determined by the initial orientation of the flamelet, while we have (from Eq. 3) $A(t_o) = 1$. The term \dot{A}_R is discussed at length

[†]If the initial flame sheet varies from one realization to the next, S_o is a random surface, and A_o is a random variable.

below. For the moment we just observe⁶ that it is zero for the case of a material surface ($w = 0$).

It is worth mentioning that the equations obtained depend on few assumptions: Eqs. (1–3) are definitions; while Eqs. (4–8) are obtained purely from geometry⁶ with the assumption that the propagation speed w is constant.

We now turn our attention to the case of a material surface ($w = 0$) which is of great theoretical interest, and is the starting point for the development of the Stochastic Flamelet Model. With $w = 0$, a “flamelet” becomes an infinitesimal material surface element, and $X(t)$ becomes the location of a fluid particle.

Since \dot{A}_R is zero (for $w = 0$), Eqs. (1), (7) and (8) can be integrated to determine the flamelet properties if $U(t)$ and $U_{i,j}(t)$ are known. Hence the first components of the model are stochastic models for these Lagrangian time series.

Space does not allow a full description of these models. Briefly, $U(t)$ is simulated by a diffusion process^{15,16} in which the diffusion coefficient depends on the dissipation $\epsilon(t)$ following the fluid particle.¹⁷ The logarithm of the dissipation is modeled as an Ornstein-Uhlenbeck stochastic process.¹⁶ The velocity gradients are modeled as the product of $\epsilon^{1/2}(t)$ and a linear combination of Gaussian stochastic processes. The linear combination is chosen so as to satisfy all constraints appropriate to homogeneous isotropic turbulence.¹⁸ The coefficients in all these models are approximately matched to correlation functions (e.g. $\langle U_{i,j}(t+s)U_{k,l}(t) \rangle$) obtained from direct numerical simulations¹⁹ of isotropic turbulence at a Taylor-scale Reynolds number of about 40.

For the initially plane, infinite, material surface $X_1(t_0) = 0$, the surface-to-volume ratio $\Sigma(x,t)$ depends solely on x_1 and t : initially it is $\Sigma(x_1, t_0) = \delta(x_1)$. The stochastic model for $U(t)$ causes $X_1(t)$ to disperse in accord with Taylor's theory:²⁰ $X_1(t)$ is Gaussian with zero mean, and its standard deviation increases first linearly with time, but ultimately as \sqrt{t} . The stochastic model for the velocity gradients is independent of U and X , and hence so also is $A(t)$. Consequently, the profiles of $\Sigma(x_1, t)$ have a Gaussian shape, their width increasing from zero, first linearly with time, and later as \sqrt{t} .

The model for $U_{i,j}(t)$ correctly results in $\langle A(t) \rangle$ being zero initially; but after a few Kolmogorov time scales, $\langle A(t) \rangle$ increases exponentially with time in accord with Batchelor's supposition.²¹ Hence the peak value $\Sigma(0, t)$ —infinite initially—first decreases as the surface disperses (but stretches little) and then increases as stretching becomes dominant, eventually increasing as e^t/\sqrt{t} .

A flame sheet ($w > 0$) differs in three ways from the material surface considered above: the flamelet does not follow a fluid particle; the density jump across the flame sheet influences U and $U_{i,j}$ (through

the associated pressure fields¹); and, the term \dot{A}_R in Eq. (8) is non-zero. In this initial study we concentrate on the third effect—area reduction caused by propagation. We consider the constant-density case (thus eliminating the second effect), and use the models for U and $U_{i,j}$ described above even for $w > 0$. (Direct numerical simulations are in progress to investigate the effect of non-zero w on these time series.) The flamelet motion (relative to the fluid) is correctly accounted for by Eq. (1).

Two mechanisms are responsible for the *area-reduction term* \dot{A}_R . Let H be the mean curvature of the surface, which is positive if the flame sheet is convex towards the reactants. Then one contribution to \dot{A}_R is ${}^6 2wHA$. The second contribution is due to cusps which can form either by the curvature becoming infinite, or by the flame-sheet propagating into itself. However caused, as cusps propagate, they tend to reduce the flame-sheet area^{4,9}—leading to a positive contribution to \dot{A}_R .

We model both contributions together by

$$\dot{A}_R(t) = C_R w A(t) \Sigma(X[t], t) \eta(t) / b(X[t], t), \quad (9)$$

where C_R is a model constant, $b(x,t)$ is the mean volume fraction of reactants, and $\eta(t)$ is an *orientation factor* defined below. This, we claim, is the simplest possible model that has the correct qualitative behavior. With the exception of the orientation factor, it is the same as that proposed by Marble & Broadwell²² in the context of turbulent diffusion flames.

One justification for the form of the model \dot{A}_R (Eq. 9) is that it accurately describes the rate of area change of a diversity of geometrically simple surfaces. We cite three examples:

- i) Consider the (disconnected) flame-sheet consisting of many infinite, plane, parallel surfaces separated by slabs of reactants and products. If the thickness of the reactant slabs is uniformly distributed (in some finite interval) then the rate of area reduction is given by Eq. (9) with $C_R \eta = 1/2$;
- ii) Consider the (disconnected) flame-sheet consisting of many equal-size spherical surfaces surrounding pockets of reactants. Then Eq. (9) with $C_R \eta = 2/3$ correctly gives the rate of area reduction. The same result (but with $C_R \eta = 1/2$) holds for circular cylindrical pockets of reactants;
- iii) Similar to ii), if the reactant pockets are equal-size regular polyhedra (e.g. cubes) then Eq. (9) holds again with $C_R \eta = 2/3$, or for cylinders of regular polygonal cross-section we find $C_R \eta = 1/2$.

While these examples bear little resemblance to the geometry of turbulent flame sheets, they nevertheless illustrate that different shapes and mecha-

nisms lead to the same formula, i.e. Eq. (9). Note that in i) the area is reduced by the mutual annihilation of colliding flame sheets; in ii) the area reduction is solely due to curvature; and, in iii) it is solely due to cusps.

As well as arising automatically in the above examples, the factor b^{-1} in Eq. (9) is suggested by a realizability condition: in the statistically homogeneous case, as reaction nears completion, Σ and b must vanish together. If, as assumed, \dot{A}_R is linearly proportional to Σ , then this realizability condition requires (as b tends to zero) that \dot{A}_R be proportional to b^{-1} . For the homogeneous case the model then predicts that Σ and b vanish together in finite time.

In the examples cited, the flame sheets are randomly orientated, and Eq. (9) holds with a constant value of $C_R\eta$. But the further example of a single, plane flame-sheet illustrates the need for the orientation factor $\eta(t)$. For this case there are no cusps or self-intersections, and the curvature is zero everywhere. Thus \dot{A}_R is zero. But it may be deduced (by a limiting process) that Eq. (9) (with $C_R\eta$ being of order unity) implies that \dot{A}_R is infinite. This problem is remedied by introducing the orientation factor $\eta(t)$.

For the plane flame, a flamelet (with properties X, A, N) has the same orientation as any other flamelet (with properties X', A', N'). Thus $N \cdot N'$ is unity. In general, if two flamelets (separated by a distance uniformly distributed in a finite interval L) are on a collision course, then the probability of their colliding in the time interval dt is

$$dP = \sqrt{2} \omega dt (1 - N \cdot N')^{1/2} / L. \quad (10)$$

This follows from simple geometric considerations. For the case of a plane flame, the two flamelets collide at infinity, and hence Eq. (10) correctly yields $dP = 0$, since $N \cdot N'$ is unity.

In the Stochastic Flamelet Model, the orientation factor $\eta(t)$ is based on the factor $(1 - N \cdot N')^{1/2}$ appearing in Eq. (10). To be precise, $\eta(t)$ is the conditional expectation of this factor, for N' being any other flamelet at the same location (on a different realization):

$$\eta(t) \equiv \langle (1 - N(t) \cdot N'(t))^{1/2} | X'(t) = X(t) \rangle. \quad (11)$$

For the statistically isotropic case (randomly orientated flamelets) the orientation factor is unity.

We have described the area-reduction model as a deterministic process: at the rate \dot{A}_R , the flamelet's area decreases smoothly and deterministically. This is the appropriate physical model if the area reduction is due to curvature. Alternatively the model could be implemented as a stochastic point process: in the time interval dt , with probability $\dot{A}_R dt$, the flamelet is annihilated (i.e. $A(t + dt) =$

0), while with probability $1 - \dot{A}_R dt$ the flamelet area is unchanged. This is the appropriate physical model if the area reduction is due to cusps. As far as single-time statistics are concerned, the result is the same however the model is implemented. The deterministic implementation is chosen since it results in smaller statistical errors in the Monte Carlo solution algorithm.

To summarize the model: stochastic processes are used to simulate the velocity $U(t)$ and its derivative $U_{i,j}(t)$ following the flamelet. Equations (1) and (7) are integrated to determine the position $X(t)$ and orientation $N(t)$ of the flamelet, while the area amplification $A(t)$ is obtained by integrating Eq. (8). The first term in Eq. (8), on average, causes an area increase, while the second is an area reduction due to curvature, cusps and self-intersections. This area reduction term is given by Eqs. (9) and (11). From the flamelet properties the surface-to-volume ratio $\Sigma(x,t)$ can be determined (Eq. 4), and hence the local burning rate $\omega(x,t)$ (Eq. 6) is obtained.

We have described the model for a single representative flamelet. To implement the model numerically we consider an ensemble of $N_f \approx 13,000$ such flamelets. The expectations—such as are required to determine $\Sigma(x,t)$ —are approximated by ensemble averages.

The burning rate $\omega(x,t)$ obtained from the flamelet model is used in the solution of the modeled transport equation¹⁵ for the joint pdf of velocity, dissipation, and reaction progress variable, c . The Monte Carlo solution of the joint pdf equation amounts to simulating the evolution of velocity, dissipation and c of an ensemble of $N_p \approx 35,000$ fluid particles. For velocity and dissipation, exactly the same stochastic models are used as for the flamelets. At (x,t) , the mean rate at which reactants ($c = 0$) burn (i.e. change to $c = 1$) is simply $\omega(x,t)$. From the joint pdf calculation, the mean volume fraction of reactants $b(x,t) = 1 - \langle c(x,t) \rangle$ is obtained and supplied to the Stochastic Flamelet Model.

Results

The Stochastic Flamelet Model in combination with the joint pdf method has been used to simulate the idealized case of an initially plane flame. The flow is statistically-stationary, homogeneous, isotropic turbulence with zero mean velocity. The turbulent kinetic energy k and the mean dissipation rate $\langle \epsilon \rangle$ are taken to be unity: hence the turbulence intensity is $u' = \sqrt{2/3}$. The Taylor-scale Reynolds number is 40, and the Kolmogorov time scale is 0.064.

At the initial time ($t = t_0 = 0$) a plane flame sheet at $x_1 = 0$ separates reactants ($c = 0, x_1 > 0$) from products ($c = 1, x_1 < 0$). We investigated two

laminar flame speeds: $w = 0.01$ and $w = 1.0$ (or $w/u' = 0.0122$ and $w/u' = 1.22$).

For the smaller laminar flame speed ($w = 0.01$) Fig. 2 shows the total flame sheet area A_T (per unit initial area) as a function of time. It may be seen that for large times ($t > 2$, say) A_T asymptotes to a value of about 300. At these times the area generation by stretching (the first term in Eq. 8) is balanced by the area reduction \dot{A}_R . But at early times ($t < 0.5$, say), because $w \Sigma$ is small, \dot{A}_R is small. Thus the flame sheet behaves much like a material surface: after a small transient ($0 \leq t \leq 0.1$, say), A_T increases exponentially with time.

Figure 3 shows the loci of the constant concentration points in the flame: $x_\alpha(t)$ is defined such that

$$\langle c(x_1 = x_\alpha[t], t) \rangle = \alpha. \tag{12}$$

Thus $x_{0.5}(t)$ is the locus of the center of the flame, and $x_{0.1}(t)$ and $x_{0.9}(t)$ are taken to mark the front and back of the flame, respectively.

It may be seen that initially ($t < 0.5$, say) the flame barely moves ($x_{0.5} \approx 0$), and its width $x_{0.1} - x_{0.9}$ grows linearly in time. Again, this is because the slowly propagating flame sheet behaves (initially) like a material surface: there is little combustion. But as time progresses and A_T grows, burning becomes significant, and the flame begins to move. At large times ($t > 2$, say) the turbulent flame speed $u_T = dx_{0.5}/dt$ (or wA_T) adopts a constant value of about 3.0, and the constant width $x_{0.1} - x_{0.9}$ is about 1.2.

The same plots for the fast laminar flame speed ($w = 1.0$) are shown in Figs. 4 and 5. Initially, A_T decreases to a minimum of 0.95, then increases rapidly, and more slowly asymptotes to a value of 3.4. The initial decrease is physically impossible and

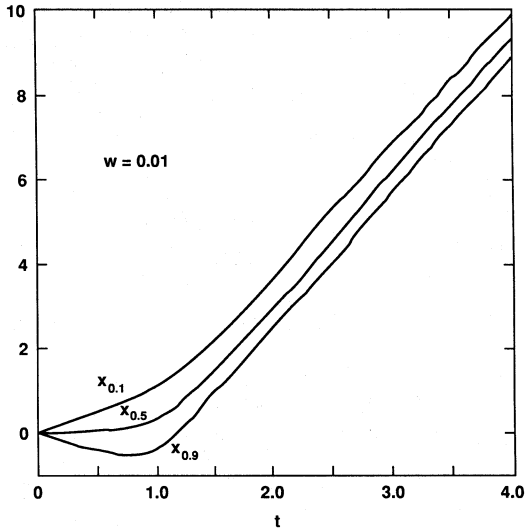


FIG. 3. Loci of points $x_{0.1}(t)$, $x_{0.5}(t)$, $x_{0.9}(t)$ at which the mean progress variable is 0.1, 0.5 and 0.9 respectively. Propagation speed $w = 0.01$.

is a defect—perhaps a small one—in the model. Even with the inclusion of the orientation factor, $\eta(t)$, at small (non-zero) times an initially plane flame develops positive area reduction \dot{A}_R faster than it is stretched by the turbulence.

In contrast to the case $w = 0.01$, Fig. 5 shows that with $w = 1.0$, significant burning starts immediately. The asymptotic value of the turbulent flame speed u_T is 3.4, while the thickness is again about 1.2.

An interesting statistic is $\langle N_1(t) \rangle$ —the component of the normal in the x_1 -direction, averaged over the

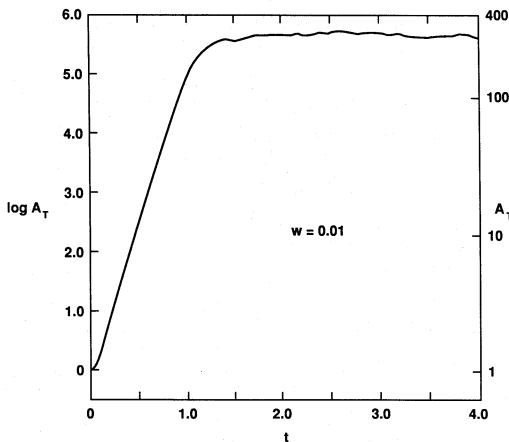


FIG. 2. Natural logarithm of flame sheet area (per initial area) against time, propagation speed $w = 0.01$.

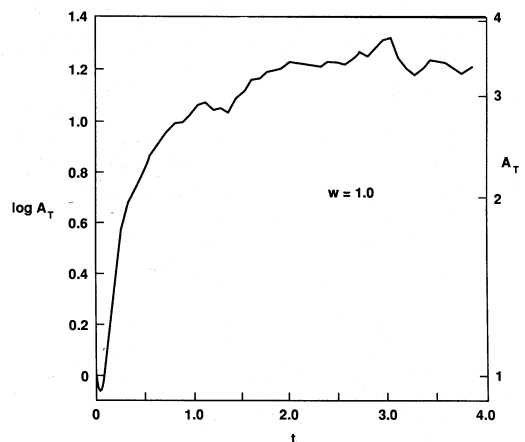


FIG. 4. Natural logarithm of flame sheet area (per initial area) against time. Propagation speed $w = 1.0$.

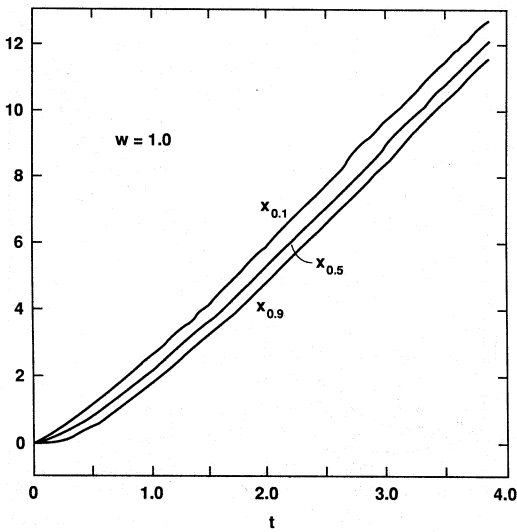


FIG. 5. Loci of points $x_{0.1}(t)$, $x_{0.5}(t)$, $x_{0.9}(t)$ at which the mean progress variable is 0.1, 0.5 and 0.9 respectively. Propagation speed $w = 1.0$.

flame sheet. Initially it is unity. For the slow flame speed ($w = 0.01$), and for a material surface ($w = 0$), after about one time unit (N_1) asymptotes to zero as the flamelets lose memory of their initial orientation. But for the faster flame speed ($w = 1.0$) the asymptotic value is 0.32. This is because flamelets moving backwards (negative N_1) or sideways ($N_1 \approx 0$) suffer greater area reduction than those moving forward ($N_1 > 0$).

Figure 6 shows profiles of the mean reaction progress variable $\langle c(x,t) \rangle$, and the surface-to-volume ratio $\Sigma(x_1,t)$ in the asymptotic state of the flame with $w = 1.0$. (For the flame with $w = 0.01$ the shapes of the profiles are similar, but Σ is larger by a factor of about 100.) The profile shapes are quite different at the front and back of the flame. At the front both Σ and $\langle c \rangle$ have long tails, while at the back Σ and $b (= 1 - \langle c \rangle)$ vanish quite abruptly. At the front, because b is small, area reduction is small, and the flame area grows by turbulent straining. Towards the center of the flame, as b becomes significant, area reduction begins to dominate causing Σ to decrease.

Discussion and Conclusions

In this work we have described and demonstrated the Stochastic Flamelet Model for turbulent premixed flames in the flamelet regime. The sample Monte Carlo calculations presented in the previous section confirm that the model and numerical algorithm provide a tractable calculation procedure

for non-stationary, inhomogeneous flames. Each of the calculations reported required about 150 CPU minutes on a minicomputer which is equivalent to 2 CPU minutes on a CRAY XMP.

As mentioned in the introduction, existing models—the Bray-Moss-Libby model,^{10,11} or the joint pdf method,¹²⁻¹⁵ for example—have difficulty in determining the local rate of burning. Perhaps this is inevitable, since these models contain no information about the flame sheet that is responsible for the fuel consumption. The Stochastic Flamelet Model, on the other hand, contains a rather natural and complete statistical description of the flame sheet—its position, orientation and area. Because of this, the essential physical processes are readily incorporated in a natural manner. Most important among these are the straining of the flame sheet, the influence of the laminar flame speed, and the area reduction caused by curvature and cusps.

This first effort leaves many improvements and extensions ahead. The models of velocity $U(t)$ and its gradient $U_{i,j}(t)$ following a flamelet require further development and validation, in particular with regard to their dependence on Reynolds number and the laminar flame speed. Direct numerical simulations will provide invaluable information for this purpose.

The essential extension of the model to the variable-density case holds both difficulty and promise. The principal difficulty is that the velocity field—especially in the vicinity of the flame sheet—is affected by the flame sheet's propagation. Hence U and $U_{i,j}$ are no longer purely turbulence quantities, but are directly affected by the flame sheet itself. Modeling aside, there is no difficulty in extending the calculation procedure to variable-density flow: indeed, previous pdf calculations of premixed flames^{13,14} have incorporated realistic density ratios.

The promise is that the additional information contained in the flamelet model may lead to im-

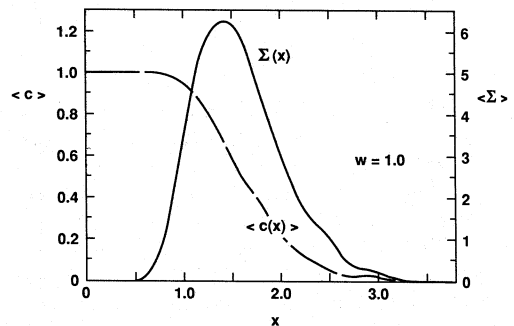


FIG. 6. Profiles of mean progress variable and surface-to-volume ratio. (The origin of x has been shifted.)

improvements in the modeling of the effect of combustion on the turbulence. A major uncertainty in both the Bray-Moss-Libby model^{10,11} and the joint pdf method¹⁴ is that the pressure fluctuations due to combustion are ignored. As observed by Pope,¹ some of these pressure effects can be directly related to flame-sheet processes.

Nomenclature

$A(t)$	flamelet area amplification factor
A_o	initial expected surface area
A_R	rate of area reduction due to cusps and curvature
$A_s(t)$	total expected surface area
A_T	total expected surface area per unit initial area
A_v	flamelet area within volume V
$b(x,t)$	mean volume fraction of reactants
C_R	model constant for area reduction
$c(x,t)$	reaction progress variable
$dA(t)$	flamelet area
dA_o	initial flamelet area
H	mean curvature
$N(t)$	unit normal vector into reactants
S_o	initial surface
t	time
t_o	initial time
$U(t)$	velocity of a flamelet
$U_{i,j}(t)$	velocity derivative $\partial u_i / \partial x_j$ following a flamelet
V	volume
$u(x,t)$	Eulerian fluid velocity field
w	surface propagation speed (here equals laminar flame speed)
$X(t)$	flamelet position
X_o	initial flamelet position
x	position (independent variable)
$\delta(x)$	three-dimensional Dirac delta function at x
$\epsilon(t)$	dissipation rate
$\eta(t)$	orientation factor
$\Sigma(x,t)$	surface to volume ratio
$\omega(x,t)$	local mean burning rate (volume burnt per unit volume per unit time)
$\langle \rangle$	mean

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REFERENCES

1. POPE, S. B.: *Ann Rev. Fluid Mech.* 19, 237 (1987).
2. ABRAHAM, J., WILLIAMS, F. A. AND BRACCO, F. V.: SAE paper 850345 (1985).
3. BRAY, K. N. C.: in *Turbulent Reactive Flows*, ed. Libby, P. A. and Williams, F. A., Springer-Verlag, 1980.
4. KARLOVITZ, B., DENNISTON, D. W. JR., KNAPPS-CHAEFER, D. H. AND WELLS, F. E.: *Fourth Symposium (International) on Combustion*, p. 613, Williams and Wilkins, Baltimore, 1953.
5. MARKSTEIN, G. M.: *Non-Steady Flame Propagation*, Macmillan, New York, 1964.
6. POPE, S. B.: *The Evolution of Surfaces in Turbulence*, *Int. J. Eng'ng. Sci.* 26, 445 (1988).
7. TABACZYNSKI, R. J., TRINKER, F. H. AND SHANNON, A. S.: *Comb. Flame*, 39, 111 (1980).
8. CLAVIN, P. AND WILLIAMS, F. A.: *J. Fluid Mech.* 90, 589 (1979).
9. THOMAS, A.: *Comb. Flame*, 65, 291 (1986).
10. BRAY, K. N. C. AND MOSS, J. B.: *Acta Astronautical* 4, 291 (1977).
11. LIBBY, P. A.: *Prog. Energy Comb. Sci.* 11, 83 (1985).
12. POPE, S. B. AND ANAND, M. S.: *Twentieth Symposium (International) on Combustion*, p. 403, The Combustion Institute, 1985.
13. POPE, S. B. AND CHENG, W. K.: *Twenty-First Symposium (International) on Combustion*, p. 1473, The Combustion Institute, 1988.
14. ANAND, M. S. AND POPE, S. B.: *Comb. Flame* 67, 127 (1987).
15. POPE, S. B.: *Prog. Energy Combust. Sci.* 11, 119 (1985).
16. KARLIN, S. AND TAYLOR, H. M.: *A Second Course in Stochastic Processes*, Academic, New York, 1981.
17. POPE, S. B. AND CHEN, Y.-L.: *Bull. Amer. Phys. Soc.* 31, 1734 (1986).
18. HINZE, J. O.: *Turbulence*, McGraw Hill, New York, 2nd. Ed., 1979.
19. YEUNG, P. K., GIRIMAJI, S. AND POPE, S. B.: *Eulerian and Lagrangian Statistics from a High-Resolution Direct Simulation of Stationary Homogeneous Turbulence*, Cornell University Report, FDA-88-02, 1988.
20. TAYLOR, G. I.: *Proc. London Math. Soc.* 20, 196 (1921).
21. BATCHELOR, G. K.: *Proc. Roy. Soc. A* 213, 349 (1952).
22. MARBLE, F. E. AND BROADWELL, J. E.: *The Coherent Flame Model of Turbulent Chemical Reactions*, TRW Report, 1977.

COMMENTS

S. Candel, *Ecole Centrale Paris, France*. I would like to point out that your review of previous work dealing with the flame area per unit volume and its dynamics was incomplete (at least in the oral presentation). This concept has been put forward by Marble and Broadwall (1977) in an unpublished but nevertheless widely known report. The concept was introduced for non-premixed flames but it has been extended by our group to premixed flame situations. These authors also pointed out the main physical mechanisms which govern the balance of flame area:

- production by stretch
- destruction by mutual annihilation
- destruction by quenching

One recent publication is contained in the Proceedings of the French-American workshop which was held in Rouen in 1987. We have applied the model to the description of ducted premixed turbulent flames and the results obtained are quite encouraging.

Various extensions of the model have also been worked out to account, e.g., 1) the quenching of flamelets by high strain rates; and 2) the existence, in certain configurations, on non-premixed and premixed flamelets as well as contact surfaces across which no reaction takes place.

Of course this comment does not deny the originality of your own work but puts your contribution in the proper perspective.

Author's Reply. As may be seen from text, the work of Marble and Broadwell (1977) is referenced in the paper. This reference also appeared on a viewgraph in the oral presentation.

The concept of a turbulent premixed flame as a propagating surface goes back at least to Damköhler (1940). Since then there have been numerous discussions in the published literature on the phenomena affecting such a surface and its propagation (Karlovitze et al.⁴ 1953, for example). A full historical account is not attempted in the paper.

The relationship between the current stochastic flamelet model and previous models based on the surface-to-volume ratio Σ is precisely the same as that between the pdf method¹⁵ and second-order turbulence closures. The stochastic model provides a complete one-point description of the surface, through the surface density function⁶ (analogous to the joint pdf). And the stochastic model can be viewed as the Monte Carlo solution of the modelled evolution equation for the surface density function (analogous to the joint pdf equation). This modelled equation can be integrated to obtain corresponding equations for mean quantities—such as Σ . Thus, when this procedure is performed, it is

found that the current area-reduction model reduces to a form similar to Marble & Broadwell's model for Σ . (Just as a modelled Reynolds stress equation can be obtained by integrating the equation for the joint pdf of velocity, and hence a comparison with existing Reynolds-stress models is possible.)

The advantage of the current stochastic flamelet model over moment closures is that it provides a much more complete description of the surface, and so allows more direct and natural modelling of the processes affecting the surface.

REFERENCE

1. DAMKÖHLER, G. (1940), *Z. Elektrochem.* 46, 601.

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A. Kerstein, *Sandia National Laboratories, USA*. Do the effects of turbulence intermittency, as incorporated into your model through the lognormality assumption, significantly influence the computed results?

Author's Reply. In the results reported, the only parameter varied is the w/u' —the ratio of the laminar flame speed to the turbulence intensity. The influence of other parameters—the variance of $\ln \epsilon$, for example—has yet to be investigated.

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R. C. Aldredge, *Princeton Univ., USA*. Please explain how the variation of the laminar burning velocity of the front (due to curvature) has been or could be taken into account in your model.

Author's Reply. In the results reported, the laminar burning velocity is taken to be constant. It is generally supposed that the laminar burning velocity w depends both on the strain-rate and on the curvature. Since the time-dependent strain-rate experienced by each flamelet is a dependent variable in the model, its effect on w is readily accounted for.

On the other hand, in the model the curvature is not known. It could be incorporated either by assuming a distribution of curvature, or by solving additional ordinary differential equations for the curvature. The latter approach requires additional stochastic models for the second derivatives of velocity—adding significant complexity to the approach.

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J. F. Driscoll, Univ. of Michigan, USA. In your model, diffusion would increase flame area (A_T) to infinity after a large time if it were not for your flame shortening mechanisms, which occur when flamelets burn out parcels between themselves or when the flame is thermodiffusively stable. However, there must be additional mechanisms that prevent excessive growth of flame area. Experiments show that A_T/A_L may only be as large as three when your flame shortening mechanisms are not present (i.e., the flame is thermodiffusively unstable and is only slightly wrinkled so flame regions never touch each other). Please comment.

Author's Reply. There are four—and, we maintain, only four—mechanism by which the area of a flamelet changes. These are:

1. straining by the fluid
2. the combination of propagation and curvature
3. cusps
4. self-intersections

For the slightly-wrinkled flames mentioned in the question, only the first two mechanisms are pres-

ent. Then, solely from geometrical considerations, it follows⁶ that rate of area increase is

$$\dot{A}/A = s_T - wH, \quad (1)$$

where s_T is the rate of strain in the tangent plane, and H is the mean curvature (which is positive if the surface is concave to the reactants).

For a statistically-stationary flame, the total surface area A_T (per unit initial area) does not change with time. Equation (1) then implies

$$\langle s_T \rangle_A = \langle wH \rangle_A, \quad (2)$$

where $\langle \rangle_A$ denotes an area-weighted mean. Consequently, assuming that $\langle s_T \rangle_A$ is positive, we deduce that the mean curvature (weighted with A and w) is positive—that is, loosely, the flame is more concave than convex. This appears to provide a sufficient explanation of the experimental observations, and additional mechanisms need not be sought.

It may be observed from Fig. 4 that for $w/n' = 1.22$, the asymptotic value of A_T is about 3.4.