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MODELLING OF FLAMELET SURFACE-TO-VOLUME RATIO IN TURBULENT PREMIXED COMBUSTION

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A model is proposed, valid in the laminar flamelet regime, for the surface-to-volume ratio of a turbulent premixed flame. The new model is in a form suitable for incorporation into an existing model of turbulent premixed combustion. Exact equations are derived which describe the dynamics of the constant-property surface representing the flame interface. Unknown terms in the exact equations are modelled for the simplified case of constant-density combustion in a specified turbulence field. Numerical solutions of the modelled equations are carried out for a one-dimensional test case. Preliminary results indicate that the model is capable of predicting effects present in turbulent flame propagation, and a parametric study shows that correct trends are observed.

Introduction

Premixed turbulent combustion is of great technological importance particularly in spark-ignition engines and in industrial safety. Experimental evidence obtained both in laboratory flames and in practical systems reveals that combustion usually takes place in thin highly-wrinkled interfaces separating reactants from products. These interfaces have the local structure of a strained laminar flame and are known as laminar flamelets. There have been several theoretical descriptions of combustion in the laminar flamelet regime, notably the model formalism due to Bray, Moss and Libby[1] and the stochastic flamelet approach of Pope and Cheng.[2] A central problem in the modelling is the treatment of the mean turbulent reaction rate. This quantity depends on the local laminar flamelet burning rate and on the flamelet surface area per unit volume. The former has been modelled by the use of a laminar flamelet library[3] to describe variations in the local burning rate due to pressure, unburned temperature and turbulent straining, while the latter has been treated in a stochastic form using the p.d.f. approach,[2] or by a phenomenological balance equation.[4–6] The stochastic approach offers advantages of generality whereas a balance equation is more easily added to an existing formulation. In premixed combustion the equations due to Franke and Peters[5] and to Maistret et al.[6] are broadly comparable in the inclusion of terms representing convection, diffusion and the effects of area production and destruction due to straining and curvature.

The present work combines the benefits of the stochastic modelling with a formulation that renders it suitable for inclusion in a conventional finite-difference code. Exact equations are derived which describe turbulent flame propagation in the laminar flamelet regime. Terms which require modelling are identified and models are obtained. Realisability is guaranteed at all stages in the modelling. The use of surface-averaging together with a Lagrangian viewpoint makes direct comparison with previous model equations[5,6] difficult. The modelled equations are solved using a simple finite-difference technique and plausible results are obtained for the idealised case of a statistically-plane flame in constant-density, stationary, isotropic turbulence. Parametric studies are carried out and qualitative comparisons made with the results of previous modelling and with experimental observation.

Theory

For the derivation of exact equations we consider the case of variable-density premixed turbulent combustion. Let $c(\underline{x}, t)$ be a reaction progress variable defined to take the value zero in reactants and unity in products. Precise definitions of c in terms of species mass fractions are discussed elsewhere.[3] Let c^* be a specified fixed value of c, for example the value of c at the inflection point of an unstrained plane laminar flame. The mean volume fraction of reactants is then given by $b(\underline{x}, t) = \Pr\{c(\underline{x}, t) < c^*\}$. Note that in the terminology of the Bray-

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Moss-Libby model the mean progress variable is $\bar{c} = \langle c \rangle = 1 - b$. The flame surface $S(t)$ is defined by all points $\underline{X}$ such that $c(\underline{X}, t) = c^*$ and is therefore a constant-property surface. In previous work[2] the flame surface has been defined as a propagating surface, but the present definition has the advantages that it is not necessarily limited to thin flames and that technical problems associated with the occurrence of cusps and self-intersections are avoided. Since $c(\underline{x}, t)$ is governed by a convection-reaction-*diffusion* equation, c is smooth and so the surface S is regular except at a finite number of critical points (at which $c(\underline{x}, t) = c^*$, $|\nabla c| = 0$). We assume that these critical points have a negligible influence on the statistics considered and hence discuss them no further.

The surface S has an expected surface area per unit volume $\Sigma(\underline{x}, t)$ whose precise definition is presented by Pope,[7] and at each point $\underline{X}$ on the surface we define the unit normal $\underline{N}(= -\nabla c/|\nabla c|$, negative so that $\underline{N}$ points into the reactants), the mean curvature H and the local propagation speed w. Note that if the surface behaves locally like an unstrained plane laminar flame then $\rho(c = c^*)w = \rho(c = 0)S_L^0$. The possibility exists for w to be a function of the local state variables and of the local turbulent flow field, but for the present work we take w to be a predefined constant.

An equation for the mean volume fraction of reactants b may be derived by considering an infinitesimal volume δV containing an infinitesimal area δA of the surface S (see Fig. 1). The mean area per unit volume and the surface mean of any quantity Q are given by

$$\Sigma = \langle \delta A \rangle / \delta V$$

$$\langle Q \rangle_s = \langle Q \delta A \rangle / \Sigma \delta V \tag{1}$$

Defining an indicator function $I(\underline{x}, t)$ taking the value unity in reactants ($c < c^*$) and zero in products ($c > c^*$) we take a volume average over δV and denote the result by i. Then $b = \langle i \rangle$. By geometry it is clear that

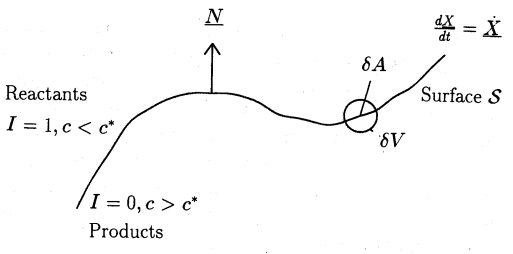


FIG. 1. The geometry of the laminar flamelet surface.

$$\frac{\partial i}{\partial t} = -\dot{\underline{X}} \cdot \underline{N} \frac{\delta A}{\partial V} \tag{2}$$

where $\dot{\underline{X}}$ is the local velocity of the surface given by the sum of the local convection velocity $\underline{U}$ and the local propagation velocity $w\underline{N}$. Thus the equation for b becomes

$$\frac{\partial b}{\partial t} = -\Sigma \langle \dot{\underline{X}} \cdot \underline{N} \rangle_s \tag{3}$$

An important consequence of this equation follows by introducing the Reynolds decomposition $\underline{U} = \langle \underline{U} \rangle + \underline{u}$ where $\underline{u}$ is the fluctuating turbulent velocity. Then $\dot{\underline{X}} = \langle \underline{U} \rangle + \underline{u} + w\underline{N}$. Substituting in (3) we have after rearrangement

$$\left(\frac{\partial}{\partial t} + \langle \underline{U} \rangle \cdot \nabla \right) b = \langle \underline{U} \rangle \cdot (\nabla b - \Sigma \underline{M}) - \Sigma \langle \underline{u} \cdot \underline{N} \rangle_s - \Sigma W, \tag{4}$$

where

$$\underline{M}(\underline{x}, t) = \langle \underline{N} \rangle_s, \tag{5}$$

and

$$W(\underline{x}, t) = \langle w \rangle_s \tag{6}$$

Every term in this equation is Galilean invariant except for the first term on the RHS, which in consequence must vanish. Therefore,

$$\underline{M} = \nabla b / \Sigma, \tag{7}$$

and we have obtained an exact expression for the surface-mean unit normal to S. This expression for $\underline{M}$ (which can also be obtained by purely geometric means) is a generalisation of the result obtained by Masuya.[10]

The exact equation for Σ has been derived elsewhere[7] and may be stated as

$$\frac{\partial \Sigma}{\partial t} + \nabla \cdot (\Sigma \langle \dot{\underline{X}} \rangle_s) = \Sigma \left\langle (\delta_{ij} - N_i N_j) \frac{\partial \dot{X}_i}{\partial x_j} \right\rangle_s. \tag{8}$$

Defining $n_{ij} = M_i M_j + 1/3 \delta_{ij}(1 - \underline{M} \cdot \underline{M})$ we may decompose the RHS of (8) as

$$\left\langle (\delta_{ij} - N_i N_j) \frac{\partial \dot{X}_i}{\partial x_j} \right\rangle_s = (\delta_{ij} - n_{ij}) \frac{\partial \langle \dot{X}_i \rangle_s}{\partial x_j} + \hat{a}_T - 2W\hat{H} \tag{9}$$

This equation defines the terms $\hat{a}_T - 2W\hat{H}$ which

are to be modelled. In the isotropic case (for which $\underline{M} = 0$, $n_{ij} = 1/3\delta_{ij}$) we obtain

$$\hat{a}_T = \hat{a} = \left\langle \frac{\partial U_i}{\partial x_j}(\delta_{ij} - N_i N_j) \right\rangle_s \tag{10}$$

which is the mean strain rate in the tangent plane of S, and

$$\hat{H} = \frac{\langle wH \rangle_s}{\langle w \rangle_s} \tag{11}$$

which is the propagation-weighted mean curvature.

The mean surface velocity is defined to be $\underline{V} = \langle \underline{U} \rangle + \langle \underline{u} \rangle_s + W\underline{M}$, and we define the convective derivative at the surface as

$$\left(\frac{D}{Dt}\right)_s = \frac{\partial}{\partial t} + \underline{V} \cdot \nabla \tag{12}$$

Thus the exact equation for Σ becomes

$$\left(\frac{D}{Dt}\right)_s \ln \Sigma = -n_{ij} \frac{\partial \langle \dot{X}_i \rangle_s}{\partial x_j} + \hat{a}_T - 2W\hat{H} \tag{13}$$

In order to express the equations for b and Σ in the same form, we make the assumptions that fluctuations in $\underline{N}$ are uncorrelated with those in $\underline{U}$ and w:

$$\langle \underline{u} \cdot \underline{N} \rangle_s = \langle \underline{u} \rangle_s \cdot \langle \underline{N} \rangle_s = \langle \underline{u} \rangle_s \cdot \underline{M}$$

$$\langle w\underline{N} \rangle_s = \langle w \rangle_s \langle \underline{N} \rangle_s = W\underline{M} \tag{14}$$

and we define

$$\alpha = 1 - \underline{M} \cdot \underline{M} \tag{15}$$

Finally, the equations for b and Σ are stated as

$$\left(\frac{D}{Dt}\right)_s b = -\alpha \Sigma W$$

$$\left(\frac{D}{Dt}\right)_s \ln \Sigma = -n_{ij} \frac{\partial V_i}{\partial x_j} + \hat{a}_T - 2W\hat{H} \tag{16}$$

which are supplemented by Eq. (7). Comparison of these equations with those arising from the phenomenological approach[5,6] is rendered difficult by the present exploitation of surface-related quantities. Since the present equations are exact a correspondence of modelled terms must exist and this is the subject of current investigation.

The form of Eq. (16) is particularly useful in addressing questions of realisability and other exact constraints. The requirement $\Sigma \geq 0$ is clearly satisfied provided only that the RHS of Eq. (16) is finite: The condition $b \geq 0$ is discussed below. More subtle is the requirement $|\underline{M}| \leq 1$, which implies $\alpha \geq 0$. For the simple case of an expanding spherical laminar flame this condition would be violated if the term in $\underline{V}$ were omitted from Eq. (16). The same term is needed to account correctly for the effect of rapid mean dilatation on Σ. An analysis of the equation for α (deduced from those for b and Σ) shows that a necessary and sufficient condition for the satisfaction of $|\underline{M}| \leq 1$ is

$$\lim_{\alpha \to 0}(\hat{a}_T - 2W\hat{H}) \geq 0 \tag{17}$$

Modelling

For convenience in the initial modelling we consider constant-density combustion in a specified turbulence field. Several quantities in the exact equations are not known *a priori* and hence require modelling. The first of these is $\langle \underline{u}_s \rangle$ which appears in $\underline{V}$ and is the surface-averaged turbulent velocity. This quantity may be interpreted as the turbulent flux of surface area for which a standard gradient-transport model is

$$\langle \underline{u} \rangle_s = -v_T \nabla \ln \Sigma \tag{18}$$

where v_T is the usual turbulent exchange coefficient given by $C_\mu k^2/\epsilon$. If the gradient-transport approach proves inadequate it is possible to solve a balance equation for $\langle \underline{u} \rangle_s$, as is already done for other turbulent fluxes in second-order closure models such as Bray-Moss-Libby.

For a material surface in isotropic turbulence ($\alpha = 1$) the straining term $\hat{a}_T$ is given by $\hat{a}_T = C_A/\tau_\eta$, where C_A has the value 0.28 obtained from direct numerical simulations of turbulence,[8] and τ_η is the Kolmogorov time scale. For a fixed surface in isotropic turbulence ($\alpha = 0$) we have $\hat{a}_T = 0$. We take the simplest model consistent with these limiting cases, namely,

$$\hat{a}_T = C_A \alpha / \tau_\eta. \tag{19}$$

It can be expected that $\hat{a}_T$ is a decreasing function of w/u_η, where u_η is the Kolmogorov velocity scale.[8] Such a dependence can in future be incorporated, once it has been quantified by direct numerical simulation.

The curvature term $\hat{H}$ is difficult to model by physical arguments, since its dependence on laminar propagation speed and on small-scale turbulent effects has yet to be investigated. Instabilities inherent in laminar propagation are also likely to be important in determining the curvature of the flame surface, particularly at small values of Reynolds

number. Previously[2,4,6] the term has been modelled by

$$2W\hat{H} = C_H \Sigma \frac{W}{b} \tag{20}$$

For the homogeneous isotropic case, the realisability condition $b \geq 0$ requires $C_H \leq 1$ (as b tends to zero). Pope and Cheng[2] took $C_H = 2/3$ which causes b to reach zero in finite time; whereas the choice $C_H = 1$ causes b to reach zero exponentially with time, and hence b remains strictly positive. Here we argue that b should be strictly positive but that it should tend to zero more rapidly than exponentially. This is achieved by the specification

$$C_H = \alpha\left\{1 - \frac{1}{3}(1 - \exp(-A\hat{R}))\right\}, \tag{21}$$

where $\hat{R} = b/(\Sigma W \tau_t)$ is the ratio of the flame-sheet to the turbulence time scales, and the constant $A = 10$. The factor α in this specification is introduced to meet the realisability requirement $\lim_{\alpha \to 0}(\hat{\alpha}_T - 2W\hat{H}) \geq 0$ mentioned above: it plays the role of the "orientation factor" of the stochastic flamelet model.[2]

Numerical Method

The model Eq. (16) together with the models detailed above are to be solved numerically by a finite difference method (as opposed to a Monte-Carlo method) with a view to future incorporation into a turbulent combustion code. The model problem is one-dimensional with open boundaries and a prescribed starting condition. The objective of the numerical calculation is to allow the turbulent flame profile to evolve from its starting conditions to a freely-propagating solution. Thus it is necessary to choose a numerical method which will capture faithfully the details of the propagation, and whose properties will not mask the nature of the physics. The need to maximise the dynamic range of the variables b and Σ leads to transformed equations for the logarithms of these quantities. Spatial discretisation was by centred differencing in order to preserve second-order accuracy and to avoid any purely numerical diffusion. This is particularly important in a problem where diffusive processes are likely to dominate the solution at least locally. Euler time differencing was employed for simplicity, and a purely explicit algorithm was adopted. Stability of the coupled system was assured by the presence of sufficient natural diffusion in the equation for Σ, there being no diffusive terms in the equation for b. End conditions for the centred differences were obtained by finding analytic solutions for b at the trailing edge and for Σ at the leading edge of the flame. A moving, variable width computational domain was adopted with nodes being added to the leading edge of the domain to accommodate the flame profile as it advanced. Nodes were removed from the trailing edge as necessary to remain within computational bounds. The use of an explicit scheme imposed restrictions on the time-step to ensure stability. A typical value of the time step proved to be about 10^{-5} for a spatial step size of 10^{-2} (in normalised coordinates), starting with a domain of 100 nodes, for which step size independent solutions were obtained and a sufficient margin of stability is guaranteed. The limitations of the finite difference approach in contrast to the Monte-Carlo method do not allow the treatment of sharp starting profiles representing a near-laminar flame but the present study centres on steady propagation rather than on the details of the evolution from the initial conditions. Parametric studies of the numerical parameters have revealed no serious pathologies. The method was coded in FORTRAN on a DECstation 3100 RISC Workstation and a typical run of 50000 time steps occupies about 5 minutes CPU.

Results and Discussion

The model code was run for a one-dimensional test case described by Pope and Cheng.[2] At time $t = 0$ the flame was assumed to exist in a field of statistically-stationary homogeneous isotropic turbulence with zero mean flow and no density variations. The initial profile was taken to be a Gaussian for Σ and an error function for b corresponding to $\underline{M} = 1$. The Taylor-scale Reynolds number was 40 and the laminar flame speed W was specified in the range 0.01 to 1.0. The turbulent kinetic energy k was taken as unity, as was the turbulent kinetic energy dissipation rate ϵ. This produced an integral time scale of unity and an rms turbulence velocity $u' = \sqrt{2/3}$. The Kolmogorov time scale τ_η was 0.064.

Results for this case are shown as a distance-time plot in Fig. 2a. for three values of the mean reactant volume fraction b. It is evident that the flame quickly settles down to a steady propagation speed and a self-preserving structure. The flame profiles in terms of the surface-to-volume ratio Σ are shown in Fig. 2b for selected times. It is clear that the profile grows rapidly as the flame area increases, developing some asymmetry towards the trailing edge. This is due to the influence of area reduction due to curvature as modeled by the expression, (20) and may be compared with the effect observed in the case of the stochastic model.[2] The total flame area is plotted in Fig. 2c as a function of time. There

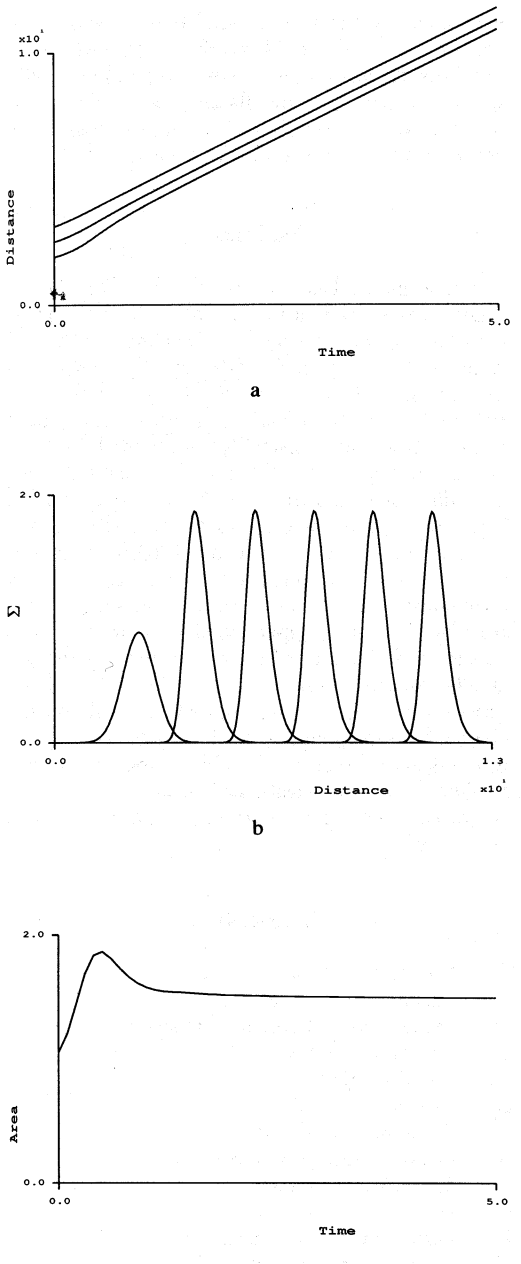


FIG. 2. Results for a typical case (Taylor-scale Reynolds number Re_λ = 40, laminar flame speed W = 1.0):

a) Distance-time plot showing the evolution to steady propagation. The three curves correspond to b = 0.1 (upper), b = 0.5 and b = 0.9.

b) Flame profiles taken at unit time intervals showing the change of shape and scale with time.

c) Total flame area as a function of time showing the rapid early increase.

is a rapid growth in area for early times followed by a slow fall back to a steady value.

Similar results are plotted in Fig. 3 for the case of laminar flame speed equal to W = 0.01. Similar qualitative behaviour is observed, but the flame takes longer to evolve to a steady state from the same starting profiles and the final flame speed is lower. Area growth is much more rapid to a considerably

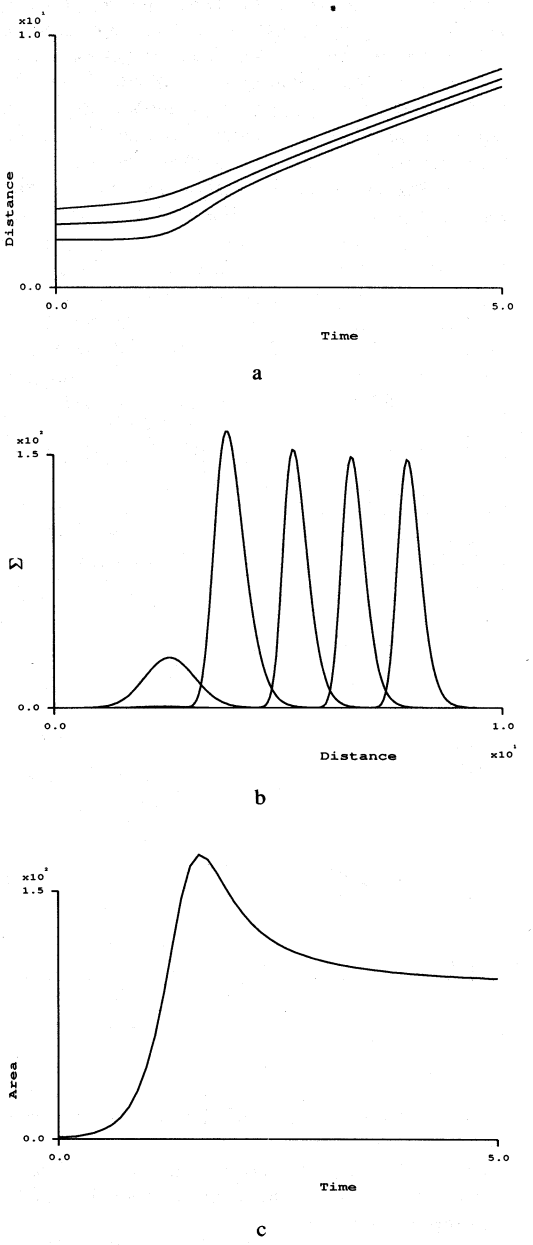
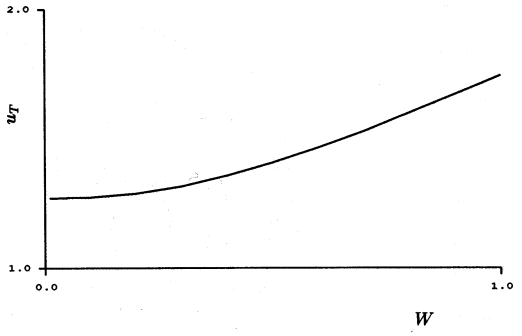


FIG. 3. Results as for Fig. 2 but with a laminar flame speed W = 0.01.

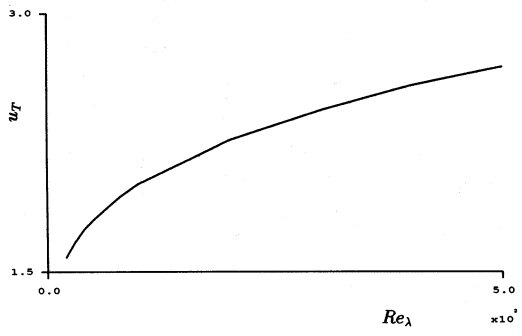
higher peak, with a slower fall back to the final value. Comparison with the stochastic flamelet model[2] reveals similar trends but considerably smaller (by 50–100%) numerical values. This is to be expected in view of the preliminary nature of the present model.

Figure 4a displays the effect on the turbulent propagation speed of varying the laminar flame speed with the Taylor-scale Reynolds number held constant. The results are satisfactory showing a variation in the appropriate sense.[9] There appears to be a tendency for the turbulent flame speed to asymptote to a constant value for small W and this is the subject of further investigation. Analysis of the model equations in this region shows that there is a finite value for u_T/u' in the limit as $W/u' \to 0$.

The effect of Reynolds number is explored in the same way in Fig. 4b. Here the laminar flame speed is held constant at $W = 1.0$ and the Reynolds number Re_λ varies from 20 to 500. Larger Reynolds numbers indicate more intense turbulence with greater wrinkling of the flame at all scales. Thus the surface-to-volume ratio may be expected to increase producing more rapid combustion.[9]



a



b

FIG. 4. Dependencies of the turbulent flame speed:

a) Turbulent flame speed u_T as a function of laminar flame speed W for a Taylor-scale Reynolds number $Re_\lambda = 40$.

b) Turbulent flame speed u_T as a function of Taylor-scale Reynolds number Re_λ for laminar flame speed $W = 1.0$.

Conclusions

A new model has been proposed for the propagation of premixed turbulent flames in the laminar flamelet regime. The model treats the variation of flame area as a primary quantity of interest and permits the calculation of the mean turbulent reaction rate in a natural manner. Exact equations have been derived and realisability conditions have been identified. Following mild simplifying assumptions, modelling of unknown terms in the equations has followed previous practice as far as possible. Numerical solutions have been obtained for a one-dimensional test problem with homogeneous isotropic turbulence and zero heat release, and the results are plausible and compare well with previous stochastic modelling. Further investigation of the parameter space is under way. The feasibility of the approach has been demonstrated and will be exploited by incorporation of the model in a more conventional (Bray-Moss-Libby type) turbulent combustion code. Density variations are catered for in the exact equations and will be incorporated in the modelling.

Nomenclature

A	Constant = 10.0
$\hat{a}_T$	Turbulent strain rate
b	Mean volume fraction of reactants
C_A	Constant = 0.28
C_H	See Eqn. (20)
C_μ	Constant = 0.09
c	Reaction progress variable
H	Mean curvature of surface S
I	An indicator function
i	Volume average of I
k	Turbulent kinetic energy
$\underline{M}$	Surface mean normal to S
$\underline{N}$	Unit normal to S
n	See Eqn. (9)
Q	A general quantity
$\hat{R}$	Ratio of turbulence time scales
Re_λ	Taylor scale Reynolds number
S	The flame surface
S_L^0	Unstrained laminar flame speed
t	Time
$\underline{U}$	Local fluid velocity
$\underline{u}$	Fluctuating turbulent velocity
u'	RMS fluctuating turbulent velocity

u_η Kolmogorov velocity
V Local surface-mean velocity
W Surface mean of w
w Local propagation speed of S
$\underline{X}$ Position vector of a point on S
$\underline{x}$ Position vector of any point

Greek:

α See Eqn. (15)
δ Kronecker delta
δA Infinitesimal area
δV Infinitesimal volume
ϵ Turbulence energy dissipation rate
ν_T Turbulent diffusivity
Σ Expected surface-to-volume ratio
τ_t Integral time scale
τ_η Kolmogorov time scale

Subscripts:

i,j Tensor suffices
s Surface-averaged quantity

Acknowledgments

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