Calculations of Burning Velocity of Turbulent Premixed Flames Using a Flame Surface Density Model*

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The objective of the present paper is to develop and validate a newly formulated Flame Surface Density (FSD) model able to predict realistic turbulent burning velocities of premixed turbulent propagating flames over a wide range of flow conditions. Non-iterative transient numerical calculations of turbulent flame propagation in one-dimensional space are carried out over a range of turbulence Reynolds number using stoichiometric methane-air mixture. It is found that the new model closely predicts experimental data of turbulent burning velocity by Abdel-Gayed et al. (1987) as well as results from KPP (Kolmogorov, Petrovski, Piskunov) analytical method. The model formulation, and subsequent results of turbulent burning velocity and combustion regimes are presented and discussed in terms of the various physical processes that control flame/flow interactions in premixed combustion.

Key Words: Premixed Combustion, Numerical Methods, Turbulence

1. Introduction

Modelling turbulent premixed flames is of interest in many areas such as in product development cycle of a spark-ignition engine or industrial fuel storage units, and in gaining fundamental knowledge of the involved physics. To date the application of Large Eddy Simulation (LES) or Direct Numerical Simulation (DNS) modelling techniques to reacting flows is limited to very simple turbulent reacting flow and geometry test cases (see, for example, Boger et al. 1998), and Favre or density weighted average predictions still continues to provide a feasible tool for engineering problems (see, for example, Miller et al. 1998).

An active area of research in modelling turbulent premixed combustion stems from the classical assumptions of a single step reaction and unity Lewis number to allow a single reduced reaction progress

variable $\tilde{c}$ ($\tilde{c}=1$ corresponding to fully burnt mixture and $\tilde{c}=0$ corresponding to unburnt mixture) to determine the mass fractions of species, and temperature. From these assumptions a critical parameter requiring modelling is the mean rate of chemical reaction $\bar{W}$. One of the main features in modelling $\bar{W}$ is the assumption of a thin laminar flame in a turbulent flow, i.e. laminar flamelet models. Classical Eddy-Break-Up (EBU) type models are probably the most commonly used models (Spalding, 1971, Magnussen and Hjertager, 1976), however, they require frequent adjustment of the model constants. On the other hand the Bray-Moss-Libby (BML) laminar flamelet model (Bray et al. 1984) has been shown to improve predictions of the turbulent burning velocity of propagating premixed flame (Patel and Ibrahim, 1999). The mean rate of chemical reaction in the BML model can be expressed as $\bar{W}=R\Sigma$ where R is the mean reaction rate of chemical reaction per unit area and Σ is the mean flamelet area to volume ratio, respectively. However, the model relies on empirical representation for Σ .

More developments have been made (Pope, 1988, Candel and Poinso, 1990, Duclos et al., 1993, Trouvé

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and Poinso, 1994) in order to improve the performance of the BML model by solving a transport equation for the flamelet surface density, Σ , where the mean rate of chemical reaction $\bar{W}$ is expressed as (Trounev and Poinso, 1994)

$$\bar{W} = \langle R \rangle_s \Sigma \quad (1)$$

where $\langle R \rangle_s$ denotes average of R over the flamelet surface area A and is defined as

$$\langle R \rangle_s = \frac{\int_0^A R dA}{A} \quad (2)$$

which can be closed as (Trounev and Poinso, 1994)

$$\langle R \rangle_s = \rho_u \langle S_c \rangle_s \quad (3)$$

where ρ_u is the density of the unburnt mixture and S_c is the flamelet speed, taken equal to the laminar burning velocity, u_L .

The closure for Σ using a transport equation may be statistically invalid (Veynante et al. 1996), however, strong relation has been shown to exist between the Σ conservation equation and its Probability Density Function (PDF) equation (Vervisch et al. 1995, and Echekki et al. 1996). Exact equations for the transport of Σ have been derived elsewhere (Pope, 1988, Candel and Poinso, 1990, Trounev and Poinso, 1994), and for the present work the Favre averaged form is adopted (Veynante et al. 1996)

$$\frac{\partial \Sigma}{\partial t} + \frac{\nabla \cdot (\bar{u} \Sigma)}{CV} + \frac{\nabla \cdot (\langle u'' \rangle_s \Sigma)}{DF} = S_\Sigma \quad (4)$$

where S_Σ is the source/sink term which can be written as (Veynante et al. 1996) :

$$S_\Sigma = \underbrace{\nabla \cdot \bar{u} - \langle n n \rangle_s : \nabla \bar{u} \Sigma}_{\bar{M}_s} + \underbrace{\langle \nabla \cdot u'' - n n : \nabla u'' \rangle_s \Sigma}_{\bar{T}_s} - \underbrace{\nabla \cdot (\langle w n \rangle_s \Sigma)}_{\bar{P}_s} + \underbrace{\langle w \nabla \cdot n \rangle_s \Sigma}_{\bar{C}_s} \quad (5)$$

where n is the unit normal vector to the flamelet pointing towards the unburned mixture, and w is the local flamelet propagation velocity relative to the mean flow velocity which can be equated to the laminar burning velocity. The terms CV , DF , $\bar{M}_s$, $\bar{T}_s$, $\bar{P}_s$, and $\bar{C}_s$ represent the convection, diffusion, stretch on the flamelet due to mean flow, turbulent flow, flame propagation, and flame curvature, respectively.

Recently, the source/sink terms, S_Σ , have been closed by either DNS (Meneveau and Poinso, 1991) or experimental (Veynante et al. 1996) findings. However, the ability of the Flamelet Surface Density (FSD) model, evolved from previous studies, to predict realistic turbulent burning velocities is yet to be investigated, which is the objective of the present work. The present work is structured as follows. Section 2 discusses and finalizes the physical sub-models for the source/sink term models. Section 3

describes the numerical technique, while results and discussion are presented in section 4, and finally the conclusions are stated in section 5.

Nomenclature

- c : Reaction progress variable
- C_m : Constant in the $\bar{M}_s$ term
- C_s : Curvature stretch term ($m^{-1}s^{-1}$)
- CV : Convection term in the Σ equation ($m^{-1}s^{-1}$)
- Da : Damköhler number
- DF : Diffusion term in the Σ equation ($m^{-1}s^{-1}$)
- e : Specific internal energy (Jkg^{-1})
- g : BML reaction rate parameter
- k : Turbulence kinetic energy (m^2s^{-2})
- K : Thermal Conductivity ($Wm^{-1}K^{-1}$)
- L : Characteristic turbulence length scale (m)
- L_y : Wrinkling length scale (m)
- $\bar{M}_s$: Mean flame stretch term ($m^{-1}s^{-1}$)
- n : Unit normal vector to flamelet
- $\bar{P}_s$: Propagation stretch term ($m^{-1}s^{-1}$)
- P : Pressure (Nm^{-2})
- R : Mean rate of chemical reaction per unit area ($kgm^{-2}s^{-1}$)
- R_L : Turbulent Reynolds number
- R_o : Universal gas constant ($Nmkmol^{-1}K^{-1}$)
- S_Σ : Source/sink term for the Σ transport equation ($m^{-1}s^{-1}$)
- t : Time (s)
- T : Temperature (K)
- $\bar{T}_s$: Turbulent flame stretch term ($m^{-1}s^{-1}$)
- u : Axial velocity (ms^{-1})
- u_L : Laminar burning velocity (ms^{-1})
- u_p : Flow velocity ahead of the flame (ms^{-1})
- u_t : Turbulent burning velocity (ms^{-1})
- w : Flamelet propagation velocity (ms^{-1})
- W : Rate of chemical reaction ($kgm^{-3}s^{-1}$)

Greek symbols

- α : Parameter in the $\bar{T}_s$ term
- β : Parameter used to calculate u_L
- γ : Parameter in the C_s term
- $\Gamma_{\bar{k}}$: ITNFS function
- ΔH : Change in specific enthalpy (Jkg^{-1})
- δ_L : Laminar flame thickness (m)
- ϵ : Rate of dissipation of k (m^2s^{-3})
- η : Kolmogorov scale of turbulence (m)
- μ : Dynamic viscosity ($kgm^{-1}s^{-1}$)
- ρ : Density (kgm^{-3})
- σ : Prandtl/Schmidt number
- σ_y : BML reaction rate parameter
- Σ : Mean flamelet surface density (m^{-1})
- τ : Heat release parameter
- $\tau_{i,j}$: Shear stress (Nm^{-2})

Subscripts

- b : Burnt mixture

i, j, k : Components of vector

o : Reference value

u : mixture

Overbars and superscripts

$\sim$: Favre averaged

$''$: Favre fluctuating quantity

$'$: Reynolds fluctuating quantity

$-$: Time averaged

Operators

$\langle \rangle_s$: Average along the flame surface

Abbreviations

BML: Bray Moss Libby

DNS: Direct Numerical Simulation

FSD: Flame Surface Density

ITNFS: Intermittent Net Flame Stretch

KPP: Kolmogorov, Petrovski, Piskunov

LES: Large Eddy Simulation

PDF: Probability Density Function

2. The FSD Model Formulation

In this section submodels for M_s , T_s , C_s , and P_s terms in (Eq. (5)) based on the most recent available experimental and numerical results are formulated and discussed.

Mean Flamelet Stretch— M_s

The mean flamelet stretch term M_s as given in Eq. (5) :

$$M_s = (\nabla \cdot \tilde{u} - \langle \mathbf{nn} \rangle_s : \nabla \tilde{u}) \Sigma \quad (6)$$

represents flamelet stretching due to mean velocity gradients. The difficulty in modelling this term arises due to a lack of knowledge on the orientation factor term $\langle \mathbf{nn} \rangle_s$. However, Veynante et al. (1996) proposed a form for $\langle \mathbf{nn} \rangle_s$ based on experimental analysis of a stabilized propane-air V-shaped flame. Here their theoretical geometrical analysis is used to model $\langle \mathbf{nn} \rangle_s$ diagonal terms, while the remaining terms are modelled using the model of Mantel and Borghi (1994), which showed reasonably good agreement with the experiments of Veynante et al. (1996). Thus,

$$\langle \mathbf{nn} \rangle_s = \begin{bmatrix} n_i n_i & n_i n_j & n_i n_k \\ n_i n_j & n_j n_j & n_j n_k \\ n_i n_k & n_j n_k & n_k n_k \end{bmatrix} = \begin{bmatrix} 0.5 & \frac{\tilde{u}_i' \tilde{u}_j''}{2\tilde{k}} & \frac{\tilde{u}_i' \tilde{u}_k''}{2\tilde{k}} \\ \frac{\tilde{u}_i' \tilde{u}_j''}{2\tilde{k}} & 0.25 & \frac{\tilde{u}_j' \tilde{u}_k''}{2\tilde{k}} \\ \frac{\tilde{u}_i' \tilde{u}_k''}{2\tilde{k}} & \frac{\tilde{u}_j' \tilde{u}_k''}{2\tilde{k}} & 0.25 \end{bmatrix} \quad (7)$$

where $\tilde{k}$ is the turbulence kinetic energy and u'' is the fluctuating velocity. The above proposal for $\langle \mathbf{nn} \rangle_s$ may be limited in validity in other configurations since it is based on experimental analysis of stabilized propane-air V-shaped flames. Nevertheless, for one-dimensional flame propagation, considered here, the

mean flow stretch can be modelled from Eq. (7) to give

$$M_s = C_m \frac{\partial \tilde{U}}{\partial x} \Sigma. \quad (8)$$

where $C_m = 0.5$ from the experiments of Veynante et al. (1996).

Turbulent Flamelet Stretch— T_s

The turbulent flamelet stretch term T_s as given in Eq. (5) :

$$T_s = \langle \nabla \cdot \mathbf{u}'' - \mathbf{nn} : \nabla \mathbf{u}'' \rangle_s \Sigma \quad (9)$$

represents flamelet stretching due to mean turbulent velocity gradients. As with the mean flow stretch term M_s the difficulty is in modelling the orientation factors $\mathbf{nn}$, which may be modelled as in Eq. (7). However, another approach, used in the present work, is to use the net flame stretch (that is the gross turbulent flame stretch effected by flame quenching) correlation of Meneveau and Poinso (1991). This correlation is a regression of their DNS results of flame-vortex interactions, and accounts for a range of scales as well as their intermittency or statistical distribution of each scale that effects the flame. Using this regression the turbulent flamelet stretch can be modelled as (Veynante et al., 1996)

$$T_s = \alpha \Gamma_{\bar{k}} \left(\frac{u'}{u_L}, \frac{L}{\delta_L} \right) \frac{\tilde{\epsilon}}{\tilde{k}} \Sigma \quad (10)$$

where $\tilde{\epsilon}$ is the dissipation rate of turbulence kinetic energy, α is a model constant having a value of 2.1 (Boudier et al. 1992), and $\Gamma_{\bar{k}}$ is the Intermittent Net Flame Stretch (ITNFS) function due to Meneveau and Poinso (1991), given in Appendix A. A central assumption in applying the ITNFS regression function to model T_s is that flame-vortex pair analysis is equivalent to flame-complete turbulent flow analysis. The variation of $\Gamma_{\bar{k}}$ or ITNFS regression function with L/δ_L for constant values of u'/u_L is shown in Fig. 1, where L is a characteristic turbulence length scale calculated from

$$L = c_{\mu}^{3/4} \frac{\tilde{k}^{3/2}}{\tilde{\epsilon}}. \quad (11)$$

It can be seen that the ITNFS function $\Gamma_{\bar{k}}$ tends to be very sensitive for values of L/δ_L greater than 100 while the sensitivity increases with higher turbulence intensity, u'/u_L .

Realistically, the model constant, α , should be a function of the turbulent flow conditions that are present ahead of the flame. The need for α to depend on flow conditions is discussed in the results section.

Flamelet Propagation Stretch— P_s

The flamelet propagation stretch term P_s as given in Eq. (5) :

$$P_s = -\nabla \cdot \langle \mathbf{wn} \rangle_s \Sigma \quad (12)$$

represents flamelet stretching resulting from the local flame propagation. This term requires modelling of

Fig. 1 Variation of ITNFS function, Γ_k , (as given in Appendix A) with u'/u_L and L/δ_L

the term $\langle w\mathbf{n} \rangle_s$ which can be approximated to $u_L \langle \mathbf{n} \rangle_s$ (Veynante et al. 1996). The modelling of $\langle \mathbf{n} \rangle_s$ is facilitated by Cant et al. (1990) who from the exact geometrical relation $\langle \mathbf{n} \rangle_s \Sigma = -\nabla \bar{c}$ obtained $\langle \mathbf{n} \rangle_s = -\nabla \bar{c} / \Sigma$. Reynolds averaged reaction progress variable, $\bar{c}$, is related to Favre averaged value of $\tilde{c}$ by (Bray, 1990)

$$\bar{c} = \frac{(1+\tau)\tilde{c}}{(1+\tau\tilde{c})} \quad (13)$$

where τ is the heat release parameter calculated from

$$\tau = \frac{\bar{\rho}_u}{\bar{\rho}_b} - 1 \quad (14)$$

where $\bar{\rho}_u$ and $\bar{\rho}_b$ are the mean density of the unburnt and burnt mixture, respectively. The spatial variation of the laminar burning velocity has been ignored since it was found to be negligible. Thus, for the present work, the flame propagation stretch term P_s can be closed as (Veynante et al. 1996)

$$P_s = u_{L,o} \frac{(1+\tau)}{(1+\tau\tilde{c})} \frac{\partial^2 \tilde{c}}{\partial x^2} \quad (15)$$

The laminar burning velocity u_L is calculated using the algebraic expression due to Metghalchi and Keck (1980) :

$$u_L = u_{L,o} \left(\frac{T_u}{T_o} \right)^{\beta_1} \left(\frac{P}{P_o} \right)^{\beta_2} \quad (16)$$

where $u_{L,o}$ is the reference laminar burning velocity (taken here equal to 0.41 m/s for stoichiometric methane/air mixture), T_o and P_o are reference temperature and pressure (taken equal to 298.15 K and 1.01 bar, respectively), T_u is the unburnt temperature

and β_1 and β_2 are constants having values 2.18 and -0.16, respectively.

Flamelet Curvature Stretch- C_s

The flamelet curvature stretch term C_s as given in Eq. (5) :

$$C_s = \langle w \nabla \cdot \mathbf{n} \rangle_s \Sigma \quad (17)$$

represents the flamelet stretching resulting from local flame curvature. The difficulty in modelling this term shifts to modelling the surface averaged flame curvature $\langle \nabla \cdot \mathbf{n} \rangle_s$. This term has been experimentally studied by Veynante et al. (1996) for stabilized propane-air V-flames. They note that this term acts as source term near the leading edge of the flame and as sink term near the trailing edge fully burnt side. To model the C_s the flame surface density, Σ , can be related to a flamelet wrinkling length scale L_y by using (Bray, 1990) :

$$\Sigma = g \bar{c} (1 - \bar{c}) / \sigma_y L_y \quad (18)$$

where g and σ_y are two reaction rate parameters which essentially account for the statistics of $\Sigma - \bar{c}$ profile and the orientation of the flamelet surface, respectively. Using Eq. (18) and assuming that the curvature term $\langle \nabla \cdot \mathbf{n} \rangle_s$ is inversely proportional to the flamelet wrinkling length scale L_y , C_s can be modelled as (Veynante et al. 1996) :

$$C_s = u_L \frac{\gamma(1+\tau\tilde{c})(\tilde{c}^o - \tilde{c})}{\tilde{c}(1-\tilde{c})} \Sigma^2 \quad (19)$$

where γ having a value of 0.4 controls the magnitude of C_s and $\tilde{c}^o$ taken equal to 0.5 controls the turn of the C_s term from source to sink.

3. Numerical Simulations

Validations of the new FSD model, formulated above, were carried out through transient calculations of turbulent premixed flame propagation in one-dimension of cartesian space. A stoichiometric methane-air mixture was used in all the calculations. The left boundary (ignition end) is closed and fixed while the right boundary is open. The length of the computational domain is 2 m.

The boundary conditions are of no flow at the closed end, and zero gradient at the open end. Initial conditions are of no mean flow with a pre-set level of turbulence. Also, ignition is simply modelled as a partially burnt mixture in the first 2% at the closed end of the total length of the computational domain.

Turbulent diffusion is modelled using the classical gradient assumption (Jones and Launder, 1972), and the solved Favre averaged conservation equations may be written as :

Mass

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x} \bar{\rho} \tilde{u} = 0 \quad (20)$$

Table 1 Values of constants used in the numerical simulations

$\sigma_{\bar{\epsilon}}$	$\sigma_{\bar{\epsilon}}$	$\sigma_{\bar{k}}$	$\sigma_{\bar{\epsilon}}$	$\sigma_{\bar{\Sigma}}$	$C_{\bar{\epsilon}1}$	$C_{\bar{\epsilon}2}$	$C_{\bar{\epsilon}3}$	C_{μ}
0.55	0.75	1.00	1.23	0.7	1.44	1.92	-0.333	0.09

Momentum

$$\frac{\partial \bar{\rho} \tilde{u}}{\partial t} + \frac{\partial}{\partial x} \bar{\rho} \tilde{u} \tilde{u} + \frac{\partial}{\partial x} \bar{\rho} \overline{u'' u''} = \frac{\partial \bar{P}}{\partial x} + \frac{\partial \tau_{xx}}{\partial x} \quad (21)$$

where

$$\tau_{xx} = -\frac{2\mu}{3} \frac{\partial \tilde{u}}{\partial x} + 2\mu \frac{\partial \tilde{u}}{\partial x} \quad (22)$$

$$\bar{\rho} \overline{u'' u''} = -\mu_t \left(2 \frac{\partial \tilde{u}}{\partial x} \right) \frac{\partial \tilde{u}}{\partial x} + \frac{2}{3} \bar{\rho} \tilde{k} \quad (23)$$

Specific Internal Energy

$$\begin{aligned} \frac{\partial \bar{p} \tilde{\epsilon}}{\partial t} + \frac{\partial}{\partial x} \bar{p} \tilde{u} \tilde{\epsilon} - \frac{\partial}{\partial x} \left(\frac{\mu_t}{\sigma_{\epsilon}} \frac{\partial \tilde{\epsilon}}{\partial x} \right) = -\frac{\partial}{\partial x} \left(K \frac{\partial T}{\partial x} \right) \\ - \frac{\partial \bar{P} \tilde{u}}{\partial x} + \frac{\partial \tau_{xx} \tilde{u}}{\partial x} - \bar{W}_c \Delta H \end{aligned} \quad (24)$$

Reaction Progress Variable

$$\frac{\partial \bar{\rho} \tilde{c}}{\partial t} + \frac{\partial}{\partial x} \bar{\rho} \tilde{u} \tilde{c} - \frac{\partial}{\partial x} \left(\frac{\mu_t}{\sigma_c} \frac{\partial \tilde{c}}{\partial x} \right) = \bar{W}_c \quad (25)$$

Flame Surface Density

$$\frac{\partial \Sigma}{\partial t} + \frac{\partial}{\partial x} \tilde{u} \Sigma - \frac{\partial}{\partial x} \left(\frac{\mu_t}{\sigma_x} \frac{\partial \Sigma}{\partial x} \right) = M_s + T_s + P_s + C_s \quad (26)$$

Turbulence Kinetic Energy

$$\frac{\partial \bar{\rho} \tilde{k}}{\partial t} + \frac{\partial}{\partial x} \bar{\rho} \tilde{u} \tilde{k} - \frac{\partial}{\partial x} \left(\frac{\mu_t}{\sigma_k} \frac{\partial \tilde{k}}{\partial x} \right) = P - \bar{\rho} \tilde{\epsilon} \quad (27)$$

where P is the production of $\tilde{k}$ due to mean velocity gradients ;

$$P = \mu_t \left(2 \frac{\partial \tilde{u}}{\partial x} \right) \frac{\partial \tilde{u}}{\partial x} \quad (28)$$

Dissipation rate of Turbulence Kinetic Energy

$$\begin{aligned} \frac{\partial \bar{\rho} \tilde{\epsilon}}{\partial t} + \frac{\partial}{\partial x} \bar{\rho} \tilde{u} \tilde{\epsilon} - \frac{\partial}{\partial x} \left(\frac{\mu_t}{\sigma_{\epsilon}} \frac{\partial \tilde{\epsilon}}{\partial x} \right) \\ = -\frac{\tilde{\epsilon}}{\tilde{k}} (C_{\bar{\epsilon}1} P - C_{\bar{\epsilon}2} \bar{\rho} \tilde{\epsilon}) \\ + C_{\bar{\epsilon}3} \bar{\rho} \tilde{\epsilon} \nabla \tilde{u} \end{aligned} \quad (29)$$

Compressibility term

The turbulent viscosity, μ_t is calculated from the turbulence kinetic energy and it's dissipation rate as (Jones and Launder, 1972)

$$\mu_t = C_{\mu} \bar{\rho} \frac{\tilde{k}^2}{\tilde{\epsilon}} \quad (30)$$

The values for the constants used in the present work are tabulated in Tabel 1 (Jones and Launder, 1972, Ahmadi-Befrui and Gosman, 1989). In addition the Equation of State is used :

$$\bar{P} = \frac{\bar{\rho} R_o \bar{T}}{\bar{M}} \quad (31)$$

The above equations are linearized using finite difference technique, in which Euler time differencing and hybrid spatial differencing are used. The linearized equations are solved using the Pressure-Implicit-Splitting-Operation PISO solver (Issa, 1986). Typical

calculation time step and grid size are 5×10^{-5} s and 5×10^{-4} m, respectively. All numerical computations have been ensured to be grid independent.

4. Results and Discussion

The presence of counter-gradient/gradient diffusion for the range of turbulence conditions covered in the present work can be obtained from the Bray number, N_B , which is defined as (Veynante et al. 1997)

$$N_B = \frac{\tau u_L}{2 \alpha_1 u'} \quad (32)$$

where α_1 accounts for the relevant turbulence length scales and is of order unity. Values of $N_B < 1$, and $N_B > 1$ indicate gradient and counter-gradient diffusion, respectively, while $N_B \approx 1$ indicates negligible scalar flux. For the turbulence conditions investigated, here, the Bray number, N_B , was found to be less than unity. This suggests that the counter-gradient diffusion effects are negligible for the flow conditions covered in the present work.

4.1 KPP analysis

The turbulent burning velocity can be obtained analytically by applying the Kolmogorov, Petrovski, Piskunov (KPP) theorem (Kolmogorov et al. 1937) to the FSD transport equation, in which the source/sink terms are modelled as described in section 2. First, it is necessary to simplify the term $\partial^2 \tilde{c} / \partial x^2$ of the P_s stretch term (Eq.(15)). This can be achieved by using the algebraic relation between the reaction progress variable and the flame surface density. This can then be used to obtain the result :

$$\frac{d^2 \tilde{c}}{dx^2} = \frac{L_y \sigma_y}{g} \frac{d^2 \Sigma}{dx^2} \quad (33)$$

where $g=1$, $\sigma_y=0.5$, and L_y is the wrinkling length scale formulated as (Bray 1990)

$$L_y = L \left(\frac{u_L}{u'} \right)^m \quad (34)$$

where $m=1$. Then, the derivation detailed in the Appendix B results in the following expression for the turbulent burning velocity

$$u_t = 2 \frac{\left[\left(\frac{\nu_t}{\sigma_x} - \frac{\gamma C^o \nu_t}{\sigma_Y} + \frac{0.11 \sigma_y u_L^2 \tilde{k}}{g \tilde{\epsilon}} \right) a \Gamma_K \frac{\tilde{\epsilon}}{\tilde{k}} \right]^{1/2}}{(1 + 2 \gamma C^o + (\gamma C^o)^2)^{1/2}} \quad (35)$$

A comparison of u_t obtained from Eq.(35) and a numerical prediction at conditions $u'/u_L=10$, $R_L=1000$ is shown in Fig. 2 . It can be seen that after a transient variation of speed at early stages of flame propagation the numerical predictions reach steady-state and result in good agreement with u_t obtained from the KPP analysis.

4.2 Turbulent burning velocity

Figure 3 shows results from typical numerical

Fig. 2 Comparison between a prediction of turbulent burning velocity obtained from KPP analytic and numerical methods ($u'/u_L=10.0$, $R_L=1\,000$)

Fig. 3 Typical predictions of reaction progress variable, rate of reaction, and flamelet surface density at time intervals of 1 ms; also shown is the variation with time of the flame speed and u_t ($u'/u_L=10.0$, $R_L=1\,000$)

Fig. 4 Comparison of predicted u_t/u_L versus u'/u_L results using the FSD model and experimental data due to Abdel-Gayed et al. (1987). — experiments, $\circ$ predictions, - - - - curve fit through predictions

predictions ($u'/u_L=10$, $R_L=1\,000$) of reaction progress variable, reaction rate, flame surface density, and velocity which highlight the initial transient and steady-state phases. Different initial values and profiles for the flame surface density, Σ , and the reaction progress variable, $\bar{c}$ in the ignition region were used to minimize the time duration to attain steady-state results, such as those shown in Fig. 3. The progress variable temporal evolution and the flow velocity ahead of the flame front were used to obtain the turbulent burning velocity, u_t by using

$$u_t = F_s - u_p \quad (36)$$

where F_s is the flame propagation speed and u_p is the steady-state flow velocity ahead of the flame. Another method was also used to confirm the values of u_t by using

$$u_t = \frac{u_p}{\tau} \quad (37)$$

where τ is the heat release parameter evaluated at the flame front. Calculated values for the turbulent burning velocity obtained from both methods were in good agreement.

Figure 4 shows a comparison between predicted and measured results of turbulent burning velocity for turbulence Reynolds numbers, R_L , of 500, 1 000, 2 000. The measured results correspond to the correlation proposed by Bray (1990) for the experimental results of Abdel-Gayed et al. (1989). It can be seen that for a fixed turbulence Reynolds number the model predic-

Fig. 5 Normalized variation of (a) M_s , (b) T_s , (c) P_s , (d) C_s , (e) CV , (f) DF , and (g) Σ terms with reaction progress variable, $\tilde{c}$ plotted at a time during steady flame propagation ($u'/u_L=2.5$, $R_L=1000$). M_s , T_s , P_s , C_s , CV , and DF normalized by $|E_s|_{\max}=7.2 \times 10^6 \text{ m}^{-1}\text{s}^{-1}$ and Σ normalized by $\Sigma_{\max}=640 \text{ m}^{-1}$

tions of turbulent burning velocity, u_t/u_L , agree well with the experiments at low turbulence intensities, u'/u_L , while at higher values the FSD model is seen to overpredict the experimental results. This apparent discrepancy may be attributed to the accuracy of the modelling of the source/sink terms in the Σ equation.

4.3 Analysis of the Σ transport equation

Figure 5 shows the variation of the M_s , T_s , P_s , C_s , CV , and DF terms for the condition $u'/u_L=2.5$ and $R_L=1000$. It can be seen that the dominant terms are M_s , T_s and C_s while the P_s and DF terms are negligible. This highlights the importance of accurately modelling the M_s , T_s and C_s terms. It was also noted that the dominance of these terms was also true for the range of turbulence conditions covered in the present work. This can be seen in Fig. 6, in which another set of result is shown for M_s , T_s , P_s , C_s , CV , and DF terms for the condition $u'/u_L=10.0$ and $R_L=1000$. Also shown in Figs. 5 and 6 is the term, $E_s=S_x-CV+DF$, and Σ . Both figures show that peak Σ occurs approximately at $\tilde{c}=0.7$ at which $E_s \approx 0$ due to steady-state. The peak location of $\tilde{c}=0.7$ agrees well with the experiments of Deschamps et al. (1996) and the DNS results of Echekki et al. (1996) which show the peak to range from $\tilde{c}=0.5$ to $\tilde{c}=0.75$.

The overpredictions seen in Fig. 4 may be due to inaccurate modelling of the C_s term. This term has

Fig. 6 Normalized variation of (a) M_s , (b) T_s , (c) P_s , (d) C_s , (e) CV , (f) DF , and (g) Σ terms with reaction progress variable, $\tilde{c}$ plotted at a time during steady flame propagation ($u'/u_L=10$, $R_L=1000$). M_s , T_s , P_s , C_s , CV , and DF normalized by $|E_s|_{\max}=4.0 \times 10^7 \text{ m}^{-1}\text{s}^{-1}$ and Σ normalized by $\Sigma_{\max}=1755 \text{ m}^{-1}$

been shown, through experimenting with liquid flames (Shy et al. 1999), to have three possible modes of variation in $\tilde{c}$ space. Mode 1 - is described by convex flamelet structure which results in C_s to be all negative. Mode 2 - is described by a combination of convex and concave flamelet structure which results in C_s to be positive and negative. Mode 3 is described by concave flamelet structure which results in C_s to be all positive. However, the curvature term in this paper only accounts for Mode 2, this is because the other two modes were identified in aqueous flames (see Shy et al. 1999) and it still remains to be seen whether these three modes do exist in gaseous premixed turbulent flames. Nevertheless, assuming that three modes do exist for the turbulence conditions covered in the present work, it could be that for u'/u_L and R_L at which overpredicted u_t were observed, the C_s term could be all destructive. Similarly, the underpredictions at low u'/u_L and R_L could be corrected with a productive C_s term. In the region of u'/u_L and R_L where close agreement of u_t was observed between the experimental and predicted the C_s term could have a combination of productive and destructive variation with $\tilde{c}$. Accounting for the other possible modes into the C_s term, as formulated in the present work, would be difficult since not much is known on the existence of the three modes of C_s over a range of

turbulence conditions. For example, Veynante et al. (1996) and Shy et al. (1999) only focus on low values of turbulence intensity, u'/u_L and Reynolds number, R_L .

Another possible inaccuracy may be in defining the value for the model constants C_m and α in the M_s and T_s stretch terms, respectively. While in the present paper the value for C_m is set at 0.5 (Veynante et al. 1996), it may be that this constant is different or depends on the turbulence condition. Similarly, a constant value of $\alpha=2.1$ (as used by Boudier et al. 1992) may change with various turbulence conditions, due to changes in flow scale, L , and turbulence intensity, u' . Thus, the M_s , T_s and C_s stretch terms are difficult to model accurately at this stage, and ideally experimental results of these terms in $\bar{c}$ space for a wider turbulence range is required.

The model for the curvature term, C_s , as used in the present paper, results in plausible predictions of $\Sigma - \bar{c}$ (see Figs. 5 and 6), as discussed earlier. However, it was noted that the Σ values were overpredicted at high u'/u_L and R_L , hence the observed overpredictions in u_t . For example, for the conditions $u'/u_L=10.0$ and $R_L=1000$, the predicted maximum value of $\Sigma=1755 \text{ m}^{-1}$ compared with experimental results of Smallwood et al. (1999) show overpredictions of approximately 1000 m^{-1} . The sensitivity of u_t to the values for γ and c^o was studied, and it was found that no significant improvements were attained in predicting u_t (the KPP analysis, see later, can also be used to show this). Now, since the sensitivity of u_t to the values for C_m , γ and c^o , has been found not to significantly improve the predictions, the remaining parameter α can be modified to take into account the discrepancy in evaluating the turbulence characteristic length scale, L from Eq.(11) (see Libby (1996)). The turbulent flamelet stretch term, T_s is proportional to the characteristic turbulence length scale, L , which is evaluated from Eq.(11). This equation is based on considering production equals dissipation of turbulence kinetic energy, hence, suggesting that this equation is valid for small turbulence scales. Therefore, the length scale formulation will be more valid at low Reynolds number than at higher values. This may explain the increasing degree of overprediction for the turbulent burning velocity, u_t , as the Reynolds number, R_L , increases (see Fig. 4). A similar argument can be used to address the increasing overprediction of u_t , for a given Reynolds number, with u'/u_L . After a series of careful sensitivity analysis, it was found that good agreements of predicted u_t with experiments is obtained when the α parameter was formulated as a function of the turbulence intensity and Reynolds number:

Fig. 7 Comparison of predicted u_t/u_L versus u'/u_L results using the FSD model with $\alpha=50/((u'/u_L)(R_L^{0.4}))$ and experimental data due to Abdel-Gayed et al. (1987). — experiments, o predictions, - - - - curve fit through predictions

$$\alpha = C(u'/u_L)^p(R_L)^q. \quad (38)$$

where C , p , and q are constants. The analysis of the turbulent burning velocity, u_t , resulted in the following values for the constants: $C=50$, $p=-1$, and $q=-0.4$. A comparison of predicted and experimental values for u_t with the modified parameter, α , as given in Eq.(38) is shown in Fig. 7. Comparing results shown in Figs. 4 and 7, it is very clear that the modified turbulent stretch parameter, α , produces more accurate results when compared with those produced when a constant value of $\alpha=2.1$ is used (Fig. 4). The $\Sigma - \bar{c}$ profiles obtained with the modified turbulent stretch parameter, α , were found to be in close agreement with the results for $\alpha=2.1$ (Figs. 5 and 6) which, as discussed, were in good agreement with experimental findings (e.g. Veynante et al. 1996, Smallwood et al. 1999). As already mentioned, results obtained with $\alpha=2.1$ overpredicted the peak values of flamelet surface density, Σ , however, with the modified α parameter (Eq.(38)) peak values for Σ were found to be lower and in better agreement with experimentally observed range of peak results between $\Sigma=200 \text{ m}^{-1}$ and 700 m^{-1} (Deschamps et al. 1996, Veynante et al. 1996, Smallwood et al. 1999). These lower values for Σ will lead to reduced mean rates of chemical reaction, $\bar{W}$, through Eq.(1), which can explain the closer agreement of predicted turbulent burning velocity results (Fig. 7).

Table 2 Criteria and burning velocity expressions for the different regimes of premixed combustion as proposed by Gülder (1990)

Range	Regime of Combustion	Burning Velocity Expression
$3200 \geq R_L \geq [1.5 \frac{u'}{u_L}]^4$	Wrinkled	$\frac{u_t}{u_L} = 1 + 0.62(\frac{u'}{u_L})^{1/2} R_L^{1/4}$
$[1.5 \frac{u'}{u_L}]^4 > R_L \geq [0.6 \frac{u'}{u_L}]^4$	Corrugated	$\frac{u_t}{u_L} = 1 + 0.62 R_L^{1/4} \exp(0.4(\frac{u'}{u_L})^{1/2})$
$R_L < [0.6 \frac{u'}{u_L}]^4$	Distributed	$\frac{u_t}{u_L} = 6.4(\frac{u'}{u_L})(\frac{u_t}{u_L})^{3/4}$

Table 3 Regimes of combustion of the predictions, and comparison between two sets of experimental results for the turbulent burning velocity (Abdel-Gayed et al. (1987) and Gülder (1990))

Run	u'/u_L	R_L	u_t/u_L (Abdel-Gayed et al (1987))	u_t/u_L (Gülder (1990))	u_t/u_L Present Work Modified α	Combustion Regime
1	2.5	500	7.45	5.64	7.1	wrinkled
2	5.0	500	8.65	8.17	8.7	corrugated
3	7.5	500	9.45	9.77	9.3	corrugated
4	10.0	500	10.05	11.38	9.9	distributed
5	2.5	1000	8.53	6.51	8.2	wrinkled
6	5.0	1000	9.91	9.53	9.4	corrugated
7	10.0	1000	11.75	11.38	11.2	distributed
8	15.0	1000	12.57	12.59	12.3	distributed
9	2.5	2000	9.78	7.56	9.2	wrinkled
10	5.0	2000	11.35	11.14	11.1	corrugated
11	10.0	2000	13.19	15.69	12.6	corrugated
12	15.0	2000	14.40	12.60	13.9	distributed
13	17.5	2000	14.88	13.09	14.5	distributed

4.4 Combustion regimes

The turbulent burning velocity, u_t , in the different regimes of combustion has been investigated by Gülder, (1990), resulting in different expressions of u_t in different regimes of combustion. The criteria used to identify the combustion regimes are tabulated in Table 2 (Gülder, 1990). According to the combustion regime criteria as proposed by Gülder, (1990), it was found that the present predictions not only covered the wrinkled and corrugated regimes, but also the distributed, or flamelet pockets, regime, hence the inclusion of the distributed regime criteria in Table 2.

The conditions investigated in the present work are reported in Table 3 along with their corresponding regime of combustion obtained from the criteria given in Table 2. Figure 8 shows the combustion regimes diagram due to Gülder (1990) superimposed with operating points from the present work, where the numbers beside the simulated points correspond to the run numbers in Table 3. In this figure, Da is the Damköhler number defined as the ratio of large scale turbulence to reaction time scale. As can be seen from Fig. 8, the present simulations cover the wrinkled, corrugated, and distributed regimes of combustion.

Also tabulated in Table 3 are two sets of experimental results for the ratio of turbulent burning veloc-

Fig. 8 Regimes of combustion due to Gülder (1990), and identification of regimes for the current predictions. The values 1 to 13 represent the number of the numerical run as tabulated in Table 3, and show the combustion regimes covered within the present study

Fig. 9 Comparison of turbulent burning velocity results obtained from KPP analysis and numerical method for a range of turbulence conditions, — KPP, $\circ$ numerical results, - - - curve fit through numerical results

ity to the laminar burning velocity u_t/u_L . It can be seen that both sets of experimental results compare reasonably well but more so in the corrugated regime. Both these sets of experimental data are based on

numerous experiments providing confidence when comparing with the results of the present work.

5. Conclusions

Transient calculations in one-dimension of steady propagating turbulent premixed flames were carried out using a newly formulated flame surface density model. A non-iterative numerical solution method was applied to solve hybrid spatial and Euler time finite difference equations. The turbulent burning velocity was obtained over a wide range of turbulence intensities $2.5 \leq u'/u_L \leq 17.5$ and Reynolds number $500 \leq R_L \leq 2000$. It was found that the model predictions agree well with the experimental results of turbulent burning velocity at low turbulence intensity, while at higher values, the model is seen to overpredict the experimental results, with the degree of overprediction increasing with Reynolds number. It was found that the model predictions were sensitive to the formulation of the turbulent flamelet stretch term, T_s . Good predictions are obtained when the T_s is formulated as:

$$T_s = \alpha \Gamma_{\bar{k}} \left(\frac{u'}{u_L}, \frac{L}{\delta_L} \right) \frac{\tilde{\epsilon}}{\bar{k}} \Sigma \quad (39)$$

with

$$\alpha = 50(u'/u_L)^{-1}(R_L)^{-0.4} \quad (40)$$

Validation of the proposed model in practical configuration is the objective of future research work.

Appendix A: ITNFS Function

A regression of the DNS results of Meneveau and Poinot (1991) results in the Intermittent Net Flame Stretch (ITNFS) function, $\Gamma_{\bar{k}}$, which has been formulated as (Duclos et al., 1993):

$$\Gamma_{\bar{k}} \left(\frac{u'}{u_L}, \frac{L}{\delta_L} \right) = \Gamma_K - \frac{3}{2} \left(\frac{L}{\delta_L} \right) \left(\frac{u'}{u_L} \right)^{-1} \ln \left(\frac{1}{1 - P_q} \right) \quad (A.1)$$

where

$$\Gamma_K = 10^{r(s, u'/u_L)} \quad (A.2)$$

$$r(s, u'/u_L) = -\frac{1}{s+0.4} \exp(-s-0.4) + [1 - \exp(-s-0.4)] \left[\sigma_1 \left(\frac{u'}{u_L} \right) s - 0.11 \right] \quad (A.3)$$

$$s = \lg \left(\frac{L}{\delta_L} \right) \quad (A.4)$$

$$\sigma_1 \left(\frac{u'}{u_L} \right) = \frac{2}{3} \left(1 - \frac{1}{2} \exp[-(u'/u_L)^{1/3}] \right) \quad (A.5)$$

$$P_q \left(\frac{L}{\delta_L}, \frac{u'}{u_L} \right) = \frac{1}{2} \{ 1 + \tanh[\text{sgn}(x)x^2] \} \quad (A.6)$$

$$x = \frac{\lg \left(\frac{u'}{u_L} \right) - g \left(\frac{L}{\delta_L} \right)}{\sigma \left(\frac{L}{\delta_L} \right)} \quad (A.7)$$

$$g \left(\frac{L}{\delta_L} \right) = \left(0.7 + \frac{1}{s} \right) \exp(-s) + [1 - \exp(-s)](1 + 0.36s) \quad (A.8)$$

$$\sigma \left(\frac{L}{\delta_L} \right) = 0.041 \lg_{10} \left(\frac{L}{\delta_L} \right) \quad (A.9)$$

Appendix B: KPP Analysis

For steady constant density one-dimensional flame propagation with the curvature term in the flame surface density equation closed as proposed by Veynante et al. (1996), the reaction progress variable and the flame surface density transport equations have to be considered. The equations can be written in a reference frame moving with the turbulent flame so that $\tilde{u} = u_t$ to yield the equations:

$$-u_t \frac{d\tilde{c}}{dx} = \frac{\nu_t}{\sigma_Y} \frac{d^2 \tilde{c}}{dx^2} - u_L \Sigma \quad (B.1)$$

$$-u_t \frac{d\Sigma}{dx} = \frac{\nu_t}{\sigma_S} \frac{d^2 \Sigma}{dx^2} + u_L \frac{d^2 \tilde{c}}{dx^2} + \alpha \Gamma_K \frac{\tilde{\epsilon}}{\bar{k}} \Sigma + \frac{u_L \gamma C^o}{\tilde{c}} \Sigma^2 \quad (B.2)$$

Introducing a solution of type $\Sigma = A \exp(-a_1 x)$ into Eq.(B.1), it can be shown that:

$$\tilde{c} = \frac{u_L A}{a_1(u_t - a_1 \nu_t \sigma_Y)} \exp(-a_1 x). \quad (B.3)$$

Equation (B.3) and the result (as discussed in the main text):

$$\frac{d^2 \tilde{c}}{dx^2} = \frac{L_y \sigma_y}{g} \frac{d^2 \Sigma}{dx^2} \quad (B.4)$$

can be substituted into Eq.(B.2) to yield the turbulent burning velocity, u_t , expression as:

$$u_t = 2 \frac{\left[\left(\frac{\nu_t}{\sigma_S} - \frac{\gamma C^o \nu_t}{\sigma_Y} + \frac{0.11 \sigma_y u_L^2 \tilde{k}}{g \tilde{\epsilon}} \right) \alpha \Gamma_K \frac{\tilde{\epsilon}}{\bar{k}} \right]^{1/2}}{(1 + 2\gamma C^o + (\gamma C^o)^2)^{1/2}} \quad (B.5)$$

More details on the KPP analysis can be obtained from Duclos et al. (1993).

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