BURNING VELOCITIES OF PROPAGATING TURBULENT PREMIXED FLAMES

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ABSTRACT

The prediction of turbulent burning velocities of premixed flames is important for many sectors of industry, for example, in the automotive sector for optimising spark-ignition engine design, and in the safe design of chemical processing plants against accedental explosions. Modelling turbulent premixed flames has received much attention over the last decade. However, such modelling attempts have generally proved to be limited to certain flow characteristics. This paper presents an assessment of two of the most commonly used premixed turbulent flame models, namely the mixing controlled Eddy Break Up (EBU) model and the Bray-Moss-Libby (BML) laminar flamelet model.

The experimental data due to Abdel-Gayed et al. (1987) are used for model validation. Previously, comparions of predictions with these numerous dimensionless experimental data have been obtained with a simple KPP analysis (Bray, 1990). In the present method, the predictions are obtained by solving transport equations for turbulent premixed flames propagating in one-dimensional spatial geometry.

Various forms of the BML laminar flamelet model based on most recent experimental reasoning are examined and validated. The results yield the typical characteristic of EBU models and show the sensitiviy of the predicted turbulent burning velocities to various formulations of the BML laminar flamelet model.

INTRODUCTION

The presence of turbulent premixed flames within a variety of industrial applications, such as in internal combustion engines and explosion studies, highligths the importance of understanding such flames. An impotant property of such flames is their turbulent burning velocity denoted here as u_t. While this quantity has been experimentally obtained by Abdel-Gayed et al. (1987) for a wide range of flow and mixture characteristics, considerable effort still continues to be diverted to modelling turbulent premixed flames.

To date, several basic concepts exist to model turbulent premixed flames, emerging mainly from the work of Damköhler (1940), Spalding (1971), and Marble and Broadwell (1977). Recently, the model due to Bray et al. (1987) has received much development attention and is commonly known as the BML laminar flamelet model.

In the BML laminar flamelet model, a starting point (Bray et al. 1987) is to formulate the mean rate of reaction, $\bar{w}$, as

$$\bar{w} = \bar{R}\bar{\Sigma} \qquad (1)$$

where $\bar{R}$ is the local mean rate of reaction per unit surface area and $\bar{\Sigma}$ is the local mean surface area to volume ratio of the flame. These two terms are modelled using algebraic expressions. Recent experiments due to Deschamps et al. (1996) and Shy et al. (1996) have provided detailed data for the BML model formulation. Also, Bray (1990) has used KPP (Kolmogorov et al., 1937) analysis on this model and good agreement is observed with the vast number of experimental data of Abdel-Gayed et al. (1987).

In this paper calculations have been carried out to assess the performance of various BML model formulations over a wide range of turbulent flow characteristics. The model validation is then carried out by comparing the predicted turbulent burning velocities with the experimental findinds due to Abdel-Gayed et al. (1987).

REACTION MODEL FORMULATION

In the present work the conservation equations for mass, momentum, turbulence, reaction progress variable, and energy are solved in a one-dimensional spatial geometry. These equations may be expressed by the general Favre averaged equation

$$\frac{\partial(\bar{\rho}\tilde{\Phi})}{\partial t}+\frac{\partial(\bar{\rho}\tilde{u}\tilde{\Phi})}{\partial x}+\frac{\partial(\bar{\rho}\widetilde{u''\Phi''})}{\partial x}=S_{\Phi} \qquad (2)$$

where $\sim$ denotes Favre average, $\bar{\rho}$ is the mean density, Φ is the dependent variable (1 for continuity, $\tilde{u}$ for momentum, $\tilde{e}$ for internal energy, $\tilde{k}$ for turbulent kinetic energy, $\tilde{\epsilon}$ for rate of turbulent energy dissipation, $\tilde{c}$ for reaction progress variable), and S_{Φ} is its source/sink term. A standard $\tilde{k}-\tilde{\epsilon}$ turbulence model (Launder and Spalding, 1972) modified for compressibilty effects is used along with gradient transport assumptions to close the conservation equations. However, the rate of reaction term $\bar{w}$ still remains to be modelled.

The commonly used EBU models express the mean rate of reaction as a function of an adjustable constant and a turbulence time scale. Here the EBU model formulates the mean rate of reaction as (Cant and Bray, 1988)

$$\bar{w}=C_{EBU}\bar{\rho}\frac{\tilde{\epsilon}}{\tilde{k}}\tilde{c}(1-\tilde{c}) \qquad (3)$$

where the adjustable constant C_{EBU} is set to 3, and $\tilde{k}/\tilde{\epsilon}$ is the turbulence time scale.

The BML laminar flamelet model expresses the mean rate of reaction as (Bray et al., 1987)

$$\bar{w}=\bar{\rho}u_L I_o\frac{g\tilde{c}(1-\tilde{c})(1+\bar{\tau})}{|\sigma_y|\hat{L}_y(1+\bar{\tau}\tilde{c})} \qquad (4)$$

where u_L is the laminar burning velocity $\hat{L}_y$ is the flamlet wrinkling length scale, I_o is a factor correcting for mean effects of strain and curvature on the laminar flame, g is a constant whose value is fixed by the Probability Density Function (PDF) of the flamelet crossing process, $|\sigma_y|$ is the cosine of the mean direction of crossing, and $\bar{\tau}$ is the heat release parameter given by

$$\bar{\tau}=\frac{\bar{\rho}_u}{\bar{\rho}_b}+1 \qquad (5)$$

where the subscripts u and b denote unburnt and burnt mixture, respectively. Thus the problem of modelling the mean rate of reaction $\bar{w}$ has converted into modelling these controlling parameters.

Here u_L is calculated using a simple algebraic expression due to Metghalchi and Keck (1980):

$$u_L=u_{LO}\left(\frac{T_R}{T_o}\right)^{\alpha}\left(\frac{\bar{P}}{P_o}\right)^{\beta} \qquad (6)$$

where u_{LO} is the reference unstrained laminar burning velocity, taken here equal to $0.41m/s$ for stoichiometric methane/air mixture, T_o and P_o are referenece temperature and pressure values (298.15K, 1.01bar), respectievly, T_R is the reactant temperature and α and β are constants with values 2.18 and -0.16, respectively.

The I_o factor is evaluated using

$$I_o=\frac{0.117K^{0.784}}{(1+\bar{\tau})} \qquad (7)$$

where K is the dimensionless Karlovitz stretch factor given by (Abdel-Gayed et al., 1987) as

$$K=0.157\left[\frac{u\prime}{u_L}\right]^2 R_L^{-0.5} \qquad (8)$$

where $u\prime$ is the r.m.s. turbulent velocity and R_L is the turbulent Reynolds number based on the integral scale of turbulence.

This expression for I_o has shown to provide reasonable agreement with I_o obtained by using the well known kolmogorov lognormal PDF of dissipation (Cant et al., 1991).

Experimental reasoning has led to the use of values of $g=1.5$ and $|\sigma_y|=0.5$ (Cant and Bray, 1988, Cant et al., 1991). However, recent experimental results due to Shy et al. (1996) indicate that the constant g should increase with the reaction progress variable (minimum and maximum values were 1.67 and and 3.16, respectively) and $|\sigma_y|=0.65$. The work of Deschamps et al. (1996) also support this since the mean flame surface density $\bar{\Sigma}$ was bias towards $\bar{c}=1$ complementing the g variation. Furthermore, studies carried out by the current authors showed that the use of the standard BML model predicted Σ peaks towards $\tilde{c}=0$ and overestimated the turbulent burning velocity u_t. To this end g may be expressed as

$$g=1+2\tilde{c} \qquad (9)$$

Based on the findings of Chew et al. (1990), Chate (1987), and Chate et al. (1988) the wrinkling length scale $\hat{L}_y$ may be expressed as (Bray, 1990)

$$\hat{L}_y=C_L L_T\left(\frac{u_L}{u\prime}\right)^n \qquad (10)$$

A value of 1 may be assigned to the constants n and C_L (Shepherd and Cheng, 1988). However, Bray (1990) suggested an algebraic expression for n based on fractal concepts of the form

$$n=6D-13 \qquad (11)$$

where D is a fractal dimension. Experimental data has been reported for D by Gouldin et al. (1988) Mantzara et al. (1989), and North and Santavicca (1990). The latter proposed that D may be given by

$$D=\frac{D_L}{\frac{u\prime}{u_L}+1}+\frac{D_T}{\frac{u_L}{u\prime}+1} \qquad (12)$$

TABLE 1. DIFFERENT FORMS OF BML LAMINAR FLAMELET MODEL.

MODEL	g	$\lvert\sigma_y\rvert$	n
BML-standard	1.5	0.5	1
BML-FORM2	$1+2\tilde{c}$	0.5	1
BML-FORM3	1.5	0.65	1
BML-FORM4	1.5	0.5	$6D-13$
BML-FORM5	$1+2\tilde{c}$	0.65	$6D-13$

where D_L and D_T are the laminar and turbulent fractal dimensions having values of 2.05 and 2.35 repectively. However, these values were not definite. Preliminary calculations suggest values for D_L and D_T of 2.19 and 2.32, repectively, which still gives reasonable results for D. All these values are based upon comparision between theoretical and experimental results for D for runs which cover a wide range of Reynolds and Damköhler numbers.

In this work systematic analysis is followed to examine the sensitivity of the BML model predictions to the model controlling parameters such as g, $|\sigma_y|$, and n. Values and expressions used for these parameters are shown in Tabel 1.

In the present work five forms of the BML laminar flamelet model are used. From this point onwards the different formulations will be reffered to as BML-standard, -FORM2, -FORM3, -FORM4, and -FORM5.

NUMERICAL SIMULATION

The finite difference form of the equations is discretised with Euler implicit time differencing and hybrid spatial differencing and the PISO solver due to Issa (1986) is used to solve the set of equations. The final code is developed and is denoted as TRF1D (Turbulent Reacting Flows in 1-Dimension).

The developed code is then applied to simulate steady turbulent flame propagtion in a simple one-dimensional geometry which may be consided as representing an axis of combustion with rectangular symmetry. The left-hand end is closed and fixed, and the other end is open.

The boundary conditons are of no flow at the closed end and zero gradient and flow boundary at the open end. Initial conditions are of no mean flow with a pre-set level of turbulence. Also, ignition is simply modelled as an intially burnt mixture in the first 1% of the total length of the computational domain. Typical calculation time step and grid size are $1\times10^{-5}s$ and $1\times10^{-4}m$, respectively, which found to provide grid independent solutions.

The prime objective of the simulations was to calculate the turbulent burning velocity u_t when the flame speed reached a steady state. This is calculated from:

$$u_t = \frac{u_p}{\bar{\tau}} \tag{13}$$

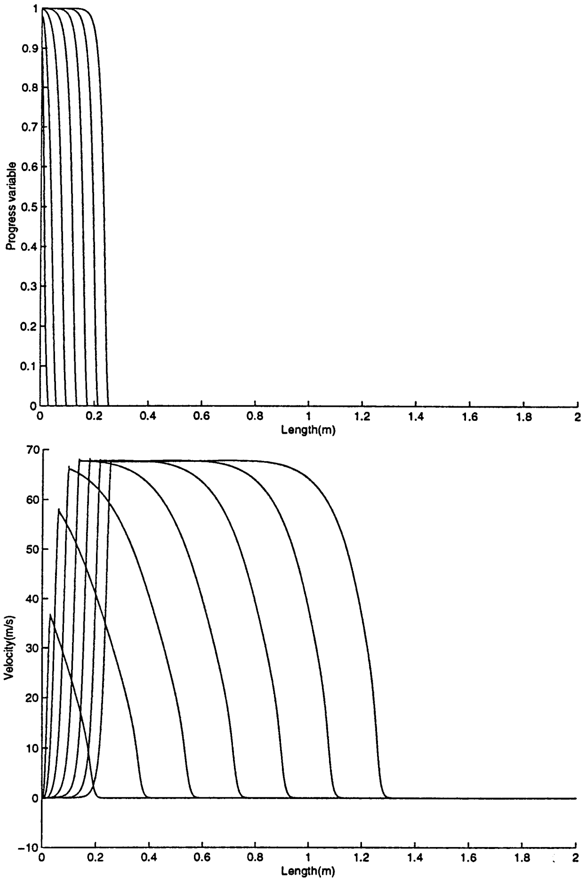

Figure 1. Typical predicted results for progress variable and velocity profile showing the steady state propagating flame at equal time intervals of $0.5ms$.

where u_p is the steady state velocity ahead of the flame. A typical predicted velocity profile showing a well defined steady state velocity u_p is given in Figure 1 along with a progress variable $\tilde{c}$ profile at times intervals of $0.5ms$.

RESULTS AND DISCUSSION

Numerical results have been obtained for the five forms of the BML flamelet model (see equations 4, 5, 6, 7, and Table 1), and an EBU model (see equation 3) for a wide range of turbulence conditions ($1.025 \leq u\prime \leq 8.2m/s$ and $500 \leq R_L \leq 3000$). Moreover, since the experimental results of Abdel-Gayed et al. (1987) have been presented in the form of a series of constant R_L lines; the present set of results have been obtained for constant R_L by pre-setting values for $u\prime$ and L_T.

Figure 2 shows a comparision between the predictions of the BML-standard model and the experimental results for R_L of 500, 1000, 2000, and 3000. It can be seen that not only are the effects of $u\prime$ and R_L on u_t/u_L reproduced, but the model also yields the gradual decay of the gradients in u_t/u_L at constant values of R_L. Systematic parametric investigation and/or the KPP analytical result (Bray, 1990) both suggest that this gradual decay is attributable to the stretch factor I_o. However, this form of the BML model over-predicts the experimental results, with the extent of over-prediction increasing as u_t/u_L increases. This gradual increase in the over-prediction may be explained through the algebraic expression for I_o which has been shown to increasingly over-predict the values of I_o obtained using the Kolmogorov pdf of dissipation, as K increases (Bray, 1990).

The results of the four alternative forms to the BML-standard model are obtained for a $R_L = 2000$, and compared with the experimental and the BML-standard model results. The results and comparisions of these four models (BML-FORM2,-FORM3,-FORM4,-FORM5) are shown in Figures 3, 4, 5, and 6, respectively. These results are then collectively shown along with the results of the EBU model in Figure 7. Similar trends are also found for different R_L values.

The results of the BML-FORM2 are shown in Figure 3. This essentailly shows the effect of g formulation on the BML model predictions. This form differs from the BML-standard model in expressing the constant g as a function of progress variable c. It can be seen that the over-predictions of the BML-standard model are reduced, and there is a closer correspondence between the experiments and predictions in relation to the gradients of the constant R_L lines (range of over-prediction approximately $5 - 12u_t/u_L$). Here, the observed trend of gradient reduction in u_t/u_L as $u\prime/u_L$ increases may be explained by the combination of I_o effects (as already explained above) and the g parameter.

The results of the BML-FORM3 model (modified $|\sigma_y|$) shown in Figure 4 yield very similar conclusions to that of the BML-FORM2 model results. However, this model does not appear to improve on the level of correspondence between the gradients of the constant R_L lines of predictions and experiments. These findings are perhaps what would be expected since $|\sigma_y|$ is inversely proportional to the mean rate of reaction $\bar{w}$ and not a function of $\tilde{c}$.

Figure 5 presents the results of the BML-FORM4 model (modified n) showing improvements from the BML-standard model. In this model the constant n is a function of laminar and turbulent fractal dimensions D_L and D_T, repectively, as shown in Table 1 and equation 12. Moreover, preliminary calculations using 2.05 and 2.35 for D_L and D_T repectively provided a near linear relation between u_t/u_L and $u_\prime/u_L$ for constant R_L. Hence, D_L and D_T are proposed new values (2.19 and 2.32, respectively) which still give results for the fractal dimension D in within the experimental results of Santavicca and North (1990).

Figure 6 shows the results obtained by combining BML-FORM2, -FORM3, and FORM4 models, hence model BML-FORM5. It can be seen that this model provides plausible correspondence with the experimental results. However, the model under-predicts u_t/u_L at low $u\prime/u_L$ (< 7) and over-predicts u_t/u_L at high u_t/u_L (> 7), but the difference is quite marginal.

An overall view of the predictions is given in Figure 7 where all the model predicted results are presented along with the results of the EBU model and compared with the experimental results. It can be noted that the EBU model does not reproduce the gradual decay of the gradient of the constant R_L line which can be attributed to the models inability to account for flame characterictics such as its thickness, speed, and stretch.

CONCLUSIONS

Calculations have been carried out to assess the performance of the EBU and BML model in predicting turbulent burning velocities of a steady propagating flame over a wide range of turbulent flow conditions. The assessment is carried out by comparing the predicted results with the experimental data due to Abdel-Gayed et al. (1987).

It is found that the EBU model does not predict the level nor gradient trend of the burning velocities with increasing turbulence level. The BML model on the other hand provides plausible results when the model controlling parameters are adjusted to take account of the recent experimental findings due to North and Santavicca (1990), Shy et al. (1996), and Deschamps et al. (1996). Validation of the modified BML model for practical applications will be the objective of future research.

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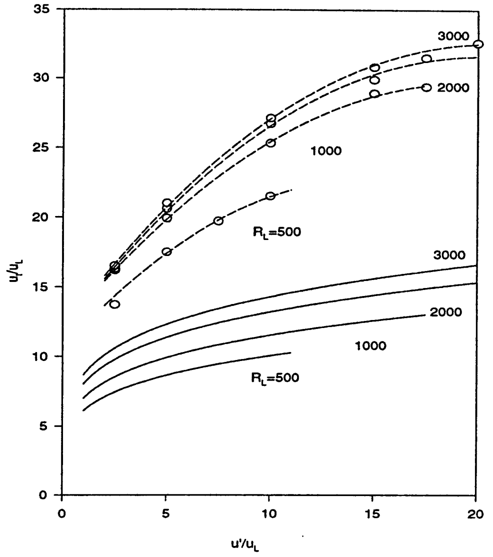

Figure 2. Comparision between BML-standard model predictions and experimental results at different R_L, - - - predictions, — experiments (Abdel-Gayed et al., 1987).

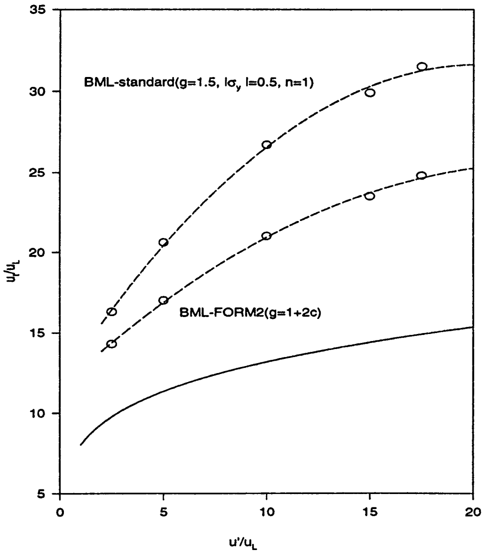

Figure 3. Effect of g parameter on BML model predictions, - - - predictions, — experiments (Abdel-Gayed et al., 1987).

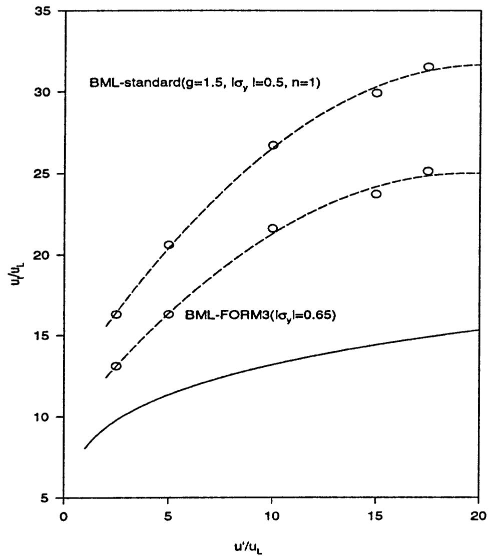

Figure 4. Effect of $|\sigma_y|$ parameter on BML model predictions, - - - predictions, — experiments (Abdel-Gayed et al., 1987).

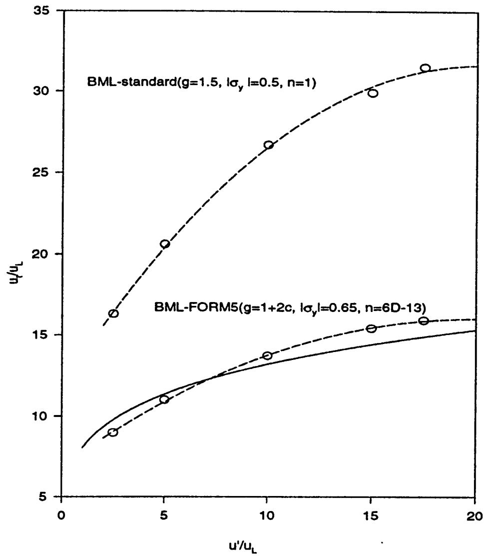

Figure 6. Comparision between a proposed BML model predictions and experimental results, - - - predictions, — experiments (Abdel-Gayed et al., 1987).

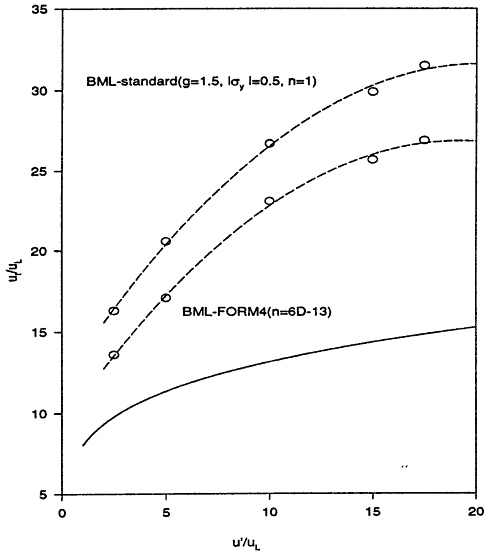

Figure 5. Effect of n parameter on BML model predictions, - - - predictions, — — experiments (Abdel-Gayed et al., 1987).

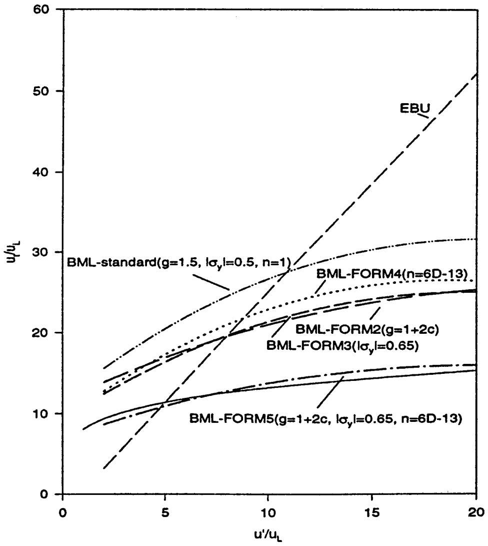

Figure 7. Comparision between the different BML models, EBU model, and experimental results, - - - predictions, — experiments (Abdel-Gayed et al., 1987).