Simulations of freely propagating turbulent premixed flames

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Simulations of Freely Propagating Turbulent Premixed Flames *

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Abstract

The propagation rate and the structure of freely propagating premixed turbulent flames are investigated using one-dimensional simulations based on the Linear-Eddy Model (LEM) (Kerstein, 1991). Extensions to earlier models were carried out to include thermo-diffusive (Lewis number), finite-rate kinetic, and heat release effects. Reasonably good quantitative agreement in predictions of turbulent flame speed with fan-stirred bomb experiments of Abdel-Gayed et al. (1984) is obtained over most of the reported u'/S_L range. The LEM predicts the initial rapid increase in u_t/S_L with u'/S_L for low u' followed by a decreasing slope in u_t/S_L with increasing u'. Here, u_t and S_L are respectively, the turbulent and laminar flame speed and u' is the turbulence intensity. Comparisons with an earlier model based on the "G-Equation" (Menon and Kerstein, 1992) are also made. The resulting propagation speeds are also in good agreement. Comparisons with weak-swirl burner experiments of stationary flames by Bedat and Cheng (1995) show that the model fails to predict the reported u_t/S_L with u'/S_L for low u' but predict a plateau in u_t/S_L as u' increases.

1 Introduction

Freely propagating premixed flames through stationary isotropic turbulence, in the absence of boundaries and external body forces though somewhat idealized, represents a fundamental flame-turbulence interaction problem encountered in many practical combustion devices such as internal combustion engines, ramjets after-burners, and industrial furnaces. Accurate prediction of characteristics such as turbulent flame speed, turbulent flame thickness, mass consumption rates, pollutant formation, turbulent flammability limits, extinction and ignition criteria are all necessary for improving the design of future combustion devices.

Prediction and analysis of propagation characteristics in complex engineering flows remains a formidable challenge. The stationary isotropic approximation simplifies the analysis of turbulence by allowing the use of well established kinetic energy inertial range scaling laws. The absence of boundaries or body forces, further simplifies the analysis and reduces the problem to a statistically one-dimensional propagation problem. The physical situation can be described as a reaction front propagating through a turbulent field separating cold reactants from hot products. The structure of the "flame brush" changes with turbulence r.m.s. intensity (u') and turbulent Damkohler number D_a = T/\tau_c. Here, \tau = l/u' is the large-eddy turnover time, l is the integral length scale, \tau_c is the chemical time scale (\tau_c \approx \delta_t/S_L) and \delta_t is the laminar flame thickness (\delta_t = \nu/S_L). At low u' and high D_a the front may be considered a singularly connected wrinkled "flamelet" with thickness equal to the laminar flame thickness. The flamelet structure is invariant to the turbulent field and thus can be considered a thin sheet with local propagation speed equal to the laminar flame speed (Peters, 1986; and Borghi, 1985). At higher u', the flame brush may
be highly convoluted and the laminar flame structure is now augmented by turbulence through the local hydrodynamic strain rate and flame surface curvature in such a way that some holes in the surface (local extinction) may appear and later disappear. The influence of strain rate and curvature are typically studied in terms of flame stretch, \( \frac{1}{2} \frac{\partial \delta A}{\partial t} \) where \( \delta A \) is an infinitesimal flame surface area, and a Karlovitz number, \( K_a \) (a non-dimensional stretch parameter). At still higher \( u' \), the flame brush may be considered a volume of disconnected flamelets having regions of steep gradients of reacting scalars and temperature (as in the situations previously described) surrounded by regions of smoothly varying reactants, products and temperature. At very high \( u' \), the concept of distributed combustion (a volumetrically distributed combustion zone with less steep gradients) has been used to describe the flame brush. The size of the small scale turbulent eddies are of the order of, or smaller than, the flame thickness and thus, are able to increase diffusion within the flame structure. This reaction zone is much thicker than the laminar flame thickness (Bedat and Cheng, 1995).

In turbulent flows where the integral length scale is slowly varying with the turbulent Reynolds number \( (Re = u' \ell / \nu) \) and \( \nu \) is the kinematic viscosity, two naturally appearing quantities which describe the influence of propagation due to burning and turbulent diffusion are the normalized turbulence intensity \( u' / S_L \) and normalized turbulent flame speed \( u_f / S_L \) (the existence of which is still being questioned). At low \( u' \), \( u_f / S_L \approx (u' / S_L)^p \) where \( p > 1 \), and at higher levels of turbulence intensity, \( u_f / S_L \approx u' / S_L \). At still higher turbulence intensities, flame stretch reduces the local burning rate and in many cases, a plateau for \( u_f / S_L \) is reached.

This functional relationship has been and continues to be the subject of many research efforts. A review of the different models of \( u_f / S_L = f(u' / S_L) \) is given by Andrews and Bradley (1975) and Gulder (1990). Experimental data for \( u_f / S_L \) has been correlated in terms of turbulent Reynolds number by Abdel-Gayed et al. (1985) and in terms of \( Re \) and Karlovitz number by Abdel-Gayed et al. (1989). Recently, new approaches to modeling the propagating flame in the different combustion regimes have been introduced. Flamelet modeling using fractal geometry has been studied (Gulder, 1990). A probability density function (pdf) method that uses a transport equation for the joint pdf of a reaction progress variable and velocity has been proposed by Pope and Anand, (1984) for modeling flamelet and distributed combustion, and a model using the joint pdf of a reaction progress variable and velocity dissipation, for combustion in the flamelet regime was proposed by Pope and Cheng, (1988). Cant et al. (1990) proposed a pdf model for the flame surface-to-volume ratio, and Cant and Bray (1988) developed a strained laminar flamelet model using an assumed pdf shape for the reaction progress variable. A one-dimensional model for the transport of flame surface density has been proposed by Fichot et al. (1993), and different closure terms appearing in flame surface density models have been studied by Duclos et al. (1993). Hakberg and Gosman (1984) developed an analytical method for deducing \( u_f / S_L \) based on a theorem of flame propagation by Kolmogorov, Petrovsky, and Piskunov. Mantel and Borghi (1994) have developed a model of pre-mixed wrinkled flame propagation based on a scalar dissipation equation. All these one-dimensional (1D) models are designed to not only to predict the fundamental characteristics of flames (such as \( u_f \)) but also to lead the way toward more comprehensive combustion modeling of complex engineering flows. In complex flows, the simplifying assumptions such as isotropic flow and statistically one-dimensional propagation may only be valid locally, as in the subgrid regions of Large-Eddy Simulation (LES) computational domains.

In this paper, we present a stochastic model for simulating freely propagating flames based on the Linear-Eddy Model (LEM) of Kerstein (1991). The model was originally developed as a mixing model and has shown capable of accurately simulating small scale mixing processes. As a pre-cursor to the LEM, the "Pair Exchange" model was used earlier by Kerstein (1986) to simulate flamelet propagation in constant density isotropic turbulence. Laminar flamelets were approximated by considering fluid cells to be a two-valued function, either fuel or product. Laminar burning proceeded by converting fuel cells adjacent to product cells, to product cells at a rate determined by the laminar flame speed and therefore, the laminar flame structure was neglected. Turbulent convection was accomplished by exchanging pairs of cells on a linear domain. The exchange process was governed by an event frequency parameter and a length scale distribution function that when combined in a stochastic simulation, yielded the correct turbulent diffusivity based on common turbulent parameters (such as \( u' \), \( \ell \) and \( Re \)). It was determined that \( u_f / S_L \) was strongly dependent on the turbulent
diffusivity and only weakly dependent on the large scale of turbulence. More recently, molecular diffusion and chemical kinetics processes of the LEM model were replaced by a flame propagation model based on the "G-equation" flamelet model (Menon and Kerstein, 1992). Results from this study showed a linear scaling between $u'/S_L$ and $u_t/S_L$ at high $u'/S_L$ consistent with experimental data. However, this approach also ignored the flame structure and is not easily extended to include Lewis number and finite-rate effects.

In this study, a simulation model is described which attempts to provide a more comprehensive treatment of the turbulence-flame interactions. The present formulation is more general in nature in that it includes molecular diffusional processes, expansion due to heat release, general finite-rate kinetics and general transport phenomena. This allows us to study the effects of these mechanisms on the propagation speed and the structure of turbulent premixed flames. Qualitative comparisons with DNS using the proposed LEM with identical chemical and turbulence parameters (Smith and Menon, 1996) have demonstrated the capabilities of LEM to capture thermo-diffusive effects in freely propagating turbulent flames in spite of the one-dimensional formulation. Specifically, the LEM correctly predicts decreasing laminar flame speeds with decreasing Lewis number and increasing turbulent propagation speeds with decreasing Lewis number. The magnitude of the change in speed was found to be similar in magnitude to the change in speed predicted by DNS of freely propagating flames.

The present approach is also compared with the more computationally efficient "G-Equation" LEM flamelet model (Menon and Kerstein, 1992) in order to investigate the regions of applicability of the "G-Equation" model. Quantitative comparisons, in terms of propagation rates and turbulent flame structure, are made with Yakhot's Renormalization Group Theory (RNG) model (1988), high Reynolds number, fan-stirred bomb experiments of Abdel-Gayed et al. (1984), and stationary weak-swirl burner experiments of Bedat and Cheng (1995).

2 Model Formulation

The LEM is used to fully characterize the effects of turbulent diffusion on the reaction-diffusion processes in the flame zone. To resolve all the length scales, the computational domain is restricted to one dimension which is considered to be a statistical ray through the local three-dimensional (3D) flame brush in the direction of mean propagation (Kerstein, 1986). The resolution within this one-dimensional domain is chosen to resolve all the relevant length scales ranging from the integral length scale $L$ to the smallest Kolmogorov eddy $\eta$ or the laminar flame thickness, $\delta_l$, whichever is smaller. Within this 1D domain, the equations describing constant pressure, adiabatic laminar flame propagation are:

$$\frac{\partial Y_k}{\partial t} = \frac{1}{\rho} \frac{\partial \rho Y_k V_k}{\partial x} + \frac{\omega_k W_k}{\rho}$$  \hspace{1cm} (1)

$$\frac{\partial T}{\partial t} = -\frac{1}{\rho c_p} \sum_{k=1}^{N} \frac{\partial T}{\partial x} \left( \frac{\partial \rho c_p}{\partial x} \right) + \frac{1}{\rho c_p} \frac{\partial}{\partial x} \left( \frac{\rho \partial T}{\partial x} \right)$$  \hspace{1cm} (2)

and the equation of state, $p = \rho T \sum_{k=1}^{N} Y_k R_u/W_k$. Here, $T$, $p$, $R_u$, and $\rho$ are respectively, temperature, pressure, universal gas constant and mass density. The $k$th species of mass fraction, molecular weight, specific heat at constant pressure, mass reaction rate, enthalpy, and diffusion velocities are respectively, $Y_k$, $W_k$, $c_p,k$, $\omega_k$, $h_k$, and $V_k$, and $N$ is the number of species. The species enthalpy is given by $h_k = \Delta h_f^o + \int_{T'}^{T} c_{p,k}(T')dT'$, where $\Delta h_f^o$ is the standard heat of formation at standard temperature, $T^o$. The mixture averaged specific heat at constant pressure and thermal conductivity are respectively, $\bar{c}_p$ and $\bar{k}$. Molecular diffusion is approximated by Fick's Law, $V_k = -\left( \frac{D_k}{Y_k} \right) (\partial Y_k/\partial x)$, where $D_k$ is the mixture averaged diffusion coefficient of species $k$. Mass errors created by using mixture averaged diffusion coefficients are absorbed into the diluent species.

LEM incorporates turbulent stirring (convection) and laminar propagation (diffusion-reaction) separately, thus the convection terms ($u \frac{\partial T}{\partial x}$ and $u \frac{\partial Y_k}{\partial x}$) are neglected in eqs. (1) and (2). In terms of laminar flame propagation, the absence of mean convection will result in the flame propagating into the reactants, with respect to a fixed frame of reference. Physically, turbulent stirring increases the propagation rate by wrinkling (increasing) the flame surface while laminar burning acts to smoothen (decrease) the flame surface.

The LEM relates fluid element diffusivity to a random walk of a marker particle. The total turbulent
diffusion of a marker particle due to the range of eddy sizes from \( l \) to \( \eta \) based on "triplet mapping" (Kerstein, 1991) is given by:

\[
D_T \approx \nu (l/\eta)^{4/3} = \frac{2}{27} \lambda \int_{\eta}^{L} \rho^2 f(l) dl.
\]

(3)

Turbulent stirring is modeled as stochastic rearrangement events which interrupt the deterministic flame propagation (solution of eqs. 1 and 2). Each rearrangement event is interpreted as the action of a single eddy on the scalar field. Three quantities govern each event: the segment (eddy) size, the location, and the rate of events. The size is determined randomly from a pdf of eddy sizes:

\[
f(l) = \frac{5}{3} \frac{l^{-8/3}}{\eta^{-8/3} - L^{-8/3}}
\]

(4)

in the range \( \eta < l < L \) (obtained from inertial range scaling (Kerstein, 1991). The event location is randomly chosen from a uniform distribution within the 1D domain, and the event rate (or frequency) is determined using an analogy between fluid dispersion in the 1D domain and turbulent diffusivity Kerstein (1991). Detailed discussions of how these parameters are determined have been reported in cited references and, therefore, are omitted here for brevity. In earlier studies, all constants appearing in the above noted scaling relations were set to unity. However, for quantitative comparison with data, calibration of these constants is required. For example, to compare LEM predictions of scalar mixing with DNS in homogeneous isotropic turbulence, the event rate was rescaled by relating the LEM diffusivity to the large-eddy turnover time in the DNS (McMurtry et al., 1994). A similar procedure is carried out in the present study.

The event rate is determined as \( \lambda \) as

\[
\lambda = \frac{54}{5} \nu Re \left[ \left( \frac{L}{\eta} \right)^{6/3} - 1 \right] \frac{1}{C_s L^3 \left[ 1 - \left( \frac{\eta}{L} \right)^{6/3} \right]}.
\]

(5)

The time interval between events is then given as \( \Delta t_{tir} = 1/\lambda X_{LEM} \). Here, the Kolmogorov length scale is determined from the familiar inertial range scaling law \( \eta = N_\eta L Re^{-3/4} \), where \( Re \) is the turbulent Reynolds number, \( \nu \) is the kinematic viscosity and \( N_\eta \) is an empirical constant estimated by Pope, (1987) to be \( \sim 13 \), by Ronney and Yakhot, (1992) to be \( 10.76 \), and by Bradley, (1992), to be 1.28 (The effect of the choice of \( N_\eta \) will be discussed later). The model constant, \( C_s \), must also be determined for the present application (discussed later).

Once the event size and location are determined and the time of the event is reached, the rearrangement event is implemented using triplet mapping (Kerstein, 1991). This mapping first creates three copies of the selected segment and then increases the spatial gradients of the copies by compressing them by a factor of three and reversing the middle copy. Finally, the original segment is replaced by the new "mapped" segment. The mapping event has several attributes analogous to turbulent convection. First, it is known that the flame sheet surface normal vector aligns with the most compressive strain rate direction which is mimicked by the compressive nature of the triplet mapping. Second, mapping increases the number of crossings of a single scalar value which may be interpreted as an increase in surface area due to flame wrinkling. Finally, turbulent scaling laws built into the model cause rate of strain and rate of growth of flame surface area to be of the correct order of magnitude (Kerstein, 1991). The ensemble of mapping events captures key mechanistic features of turbulent stirring despite temporally discrete representation of a time continuous process. Furthermore, omission of flame surface displacement in the other two directions (since the present model is 1D) has been shown to cause significant errors only at very low turbulence intensities where a single flame persists instead of multiple flames (Kerstein, 1986).

Propagation of a premixed flame through an isotropic turbulent field is simulated by solving eqs. (1-5) on an equally spaced discretized line. Using backward-euler time integration, second-order-accurate finite-differencing for the derivatives, and a partial decoupling strategy for the source terms (Calhoun et al., 1994), the equations are marched time accurately at the diffusion time step until a statistically steady state is reached. Volumetric expansion due to heat release is implemented by expanding each linear eddy cell on the 1D line by an amount \( \rho^n / \rho^{n+1} \) where \( \rho^n \) and \( \rho^{n+1} \) are, respectively, the density of the \( i \)th cell at the \( n \) and \( n+1 \) time integration level. The domain containing the expanded cells is regridded so that each cell is returned to its initial volume. This increases the total number of cells; however, to maintain the same number of cells throughout the simulation (a simplification that will be discarded in
the future), a number of cells equal to the increase in
the number of cells are truncated from the burnt side
of the flame. Truncation is justified because the flame
brush only occupies a fraction of the domain and
propagates only into the reactant mixture. Statistics
describing the rate of propagation and the structure
of the flame brush are only meaningful in the active
regions of combustion (i.e. upstream of the location
where cells are truncated from the domain). Since
volumetric expansion is decoupled from the diffusion-
reaction equations, accuracy in calculating the laminar
flame speed is ensured by requiring adequate reso-


nution of the flame and is determined by comparing
\[ SC = \frac{\int_{-\infty}^{\infty} w_R dx}{\Delta t} \]
and
\[ SP = \Delta x_{Y_R=0.5}/\Delta t, \]
where \( w_R \) is the reactant reaction rate, \( \Delta x \) is the
reactant mass consumption rate and \( SP \) is the flame
speed based on propagation rate of a reference mass
fraction value, \( Y_R = 0.5 \), where \( Y_R = Y_k/\gamma_0 \) and \( \gamma_0 \)
is the initial mass fraction of species \( k \).

The \( G-Equation \) LEM models laminar burning (de-


scribed previously by eqs. 1 and 2) by the propagation
equation:

\[ \frac{\partial G}{\partial t} = S_L|\nabla G|. \]  (6)

This eq. tracks the propagation of a single value of
"G" between \( G_{fuel} \leq G \leq G_{prod} \), where \( G_{fuel} = 1 \)
and \( G_{prod} = 0 \). \( G_0 \) is a prespecified level surface
representing the flame. Therefore, flame propagation
is described by one scalar instead of \( N + 1 \) (Menon
and Kerstein, 1992). The flame speed \( S_L \) is also a
prespecified constant. Since there is no mathematical
description of expansion due to heat release in eq. (6),
expansion is implemented in terms of a physical
interpretation of its effect on the "G" field. The
algorithm for thermal expansion (described above)
is not appropriate here since the \( G-Equation \) has
no flame structure and therefore, no physical mech-
anism to compensate for the scalar profile broad-
ening effect due to expansion. Therefore, expansion
is implemented by first prescribing a reference
value \( G_{exp} \) that defines a transition from fuel to
product. After each time step, each new cell value,
\( G_{i+1} \), is compared to the old value, \( G_i \). If the ref-
ence value is crossed during that time step, all
the heat is released, the cell is set to \( G_{prod} \) and a
number \( (N_{exp} - 1) \) of new \( G_{prod} \) cells are added.
Here \( N_{exp} \) is the nearest integer ratio of \( TP/TF \),
where \( TP \) is the product temperature and \( TF \) is the
fuel temperature. This method artificially truncates
the scalar profile, increasing the gradient and there-


Increasing burnt cells increases relative spacing be-


tween to adjacent flames. An additional error is intro-
duced when \( TP/TF \) is not an integer value; however,
it has been determined that the flame front propa-
gation rate is relatively insensitive to the amount
of expansion, so the algorithm which correctly predicts
the repulsion speed of two adjacent flames appears
adequate.

Yakhot's RNG model is an analytical expression for
the turbulent flame speed as a function of turbulence
intensity \( (u'/S_L = exp[u^2/u^2]) \). It was derived from
the \( G-Field \) Equation (Kerstein et al., 1988) which
describes the propagation of a thin flame by the ac-
tions of convection and normal burning. The model
assumes no flame structure and is applicable only in
the flamelet combustion regime, however, it has been
shown that the model compares well with experimen-
tal data in the low to moderately high \( u'/S_L \) range.
In addition, the model predicts an increasing slope (at
low \( u'/S_L \)) and then decreasing slope (at high \( u'/S_L \))
in the normalized turbulent flame speed curve. Equa-
tion 6 was also obtained from the \( G-Field \) Equation
which makes the RNG model an appropriate choice
for comparisons with \( G-Equation \) LEM and the finite-
rate model in the flamelet regime. The RNG model
does not take into account \( D_k \) or \( K_k \) effects and
therefore can not predict extinction, however, Ron-
ney et al., (1992) have extended the model to include
flame broadening effects at high \( Re \). We will only
compare with the model in its original form in this
paper.
3 Results and Discussion

To simulate a stationary flame, a moving observation window is defined (shown in Fig. 1a) that translates with the flame brush from its original position to maintain approximately the same relative position between flame center and observation window (even though the flame propagates freely into the reactants). The extent of the flame brush is defined as the width of the domain from the "first" flame to the "last" flame with the flame center defined as the geometric center of the flame brush. The flame front location is determined by tracking a reference mass fraction \( Y_R = 0.5 \), that has been normalized by the initial reactant mass fraction, \( Y_0 \). As the front propagates into the reactants, and its position relative to the upstream computational boundary becomes less than a specified amount (usually one integral length scale), the observation window is shifted an equal amount to maintain approximately the same relative position. This shift requires eliminating cells from the burnt side (outflow) and adding new cells at the reactant (inflow) boundary. It was determined earlier by Menon and Kertein (1992), and in the present study, that this shift does not affect the statistics used to analyze the results. All statistics are obtained relative to the flame center. Figure 1b shows a "snapshot" of the flame brush. The individual profiles of \( Y_R \) represent individual flames. Note the evidence of stirring by the jagged sections of the profiles at some locations and the action of molecular diffusion by the smoothness of other profiles. Also note that the relative distance between individual flames is random in appearance.

Two chemical mechanisms are employed in this study. The first is the four-step reduced methane-air mechanism of Peters (1991):

\[
\begin{align*}
CH_4 + 2H &= CO + 4H_2 \\
CO + H_2O &= CO_2 + H_2 \\
H + H + M &= H_2 + M \\
O_2 + 3H_2 &= 2H + 2H_2O.
\end{align*}
\]

that contains eight species; \( CH_4, H_2, O_2, H, CO, CO_2, H_2O, \) and \( N_2 \) (inert). The four reversible reaction rates are functions of the elementary reaction rates deduced from a forty-equation skeletal mechanism. The thermodynamic and transport data were taken directly from the CHEMKIN-II (Kee et al., 1992) database. The method of evaluating thermodynamic properties such as \( c_p, h_k, \) and mixture averaged transport coefficients such as \( D_k, \xi, \) and \( \kappa \) are outlined in CHEMKIN-II, and Dufour and Soret diffusion effects have been neglected. Computational efficiency is significantly improved by "lining" the transport coefficient equations directly into the code. This has been adopted for the four-step mechanism results presented here.

Laminar flame speeds for lean to moderately rich mixtures are presented in fig. 2a, and flame thickness data based on thermal thickness (defined as \( \delta_h = (T_p - T_f)/(dT/dx)_{max} \)) and based on temperature profile (defined as \( \delta_T \)) are presented in fig. 2b. The LEM predictions of laminar flame properties (the simulation is carried out without turbulent stirring) are compared with the CHEMKIN-II PREMIX code, calculations by Peters (1991) and laminar flame bomb experiments by Andrews and Bradley (1972). The LEM and CHEMKIN-II predictions of flame speed, \( \delta_h \) (fig. 2b), and \( \delta_T \) (not shown) are in excellent agreement. These results demonstrate that the decoupling of expansion due to heat release in the diffusion-reaction equations does not create any significant error in the flame speed or flame thickness calculations. The differences in flame speed between the results and Peters are mainly due to the manner in which the equilibrium concentrations are obtained. Thus this is not related to the LEM implementation of the mechanism or to any deficiency in the solution of the diffusion-reaction equations, (1) and (2). The reduced four-step mechanism has a relatively thick recombination zone which causes \( \delta_T \) predicted by the four-step mechanism to be larger than the experimental results. Both LEM and CHEMKIN-II predict this behavior. However, \( \delta_h \) compares much more closely to the experimental data (fig. 2b). Note that it is common practice to define the laminar flame thickness in terms of the laminar flame speed and the kinematic viscosity \( (\bar{\nu} = \nu/\bar{S}_L) \). A flame thickness defined in this manner is typically less than the thermal thickness or the temperature profile thickness.

The second mechanism studied is a single-step global decomposition mechanism; \( R \rightarrow P \) (reactants form products) (discussed in Williams, 1985). In this case, the chemistry is described by an overall activation energy, pre-exponential factor, and product temperature. The mass rate of destruction of the normalized reactant that ranges from \([1 \rightarrow 0]\) is; \( \dot{\omega}_R = -\rho Y_R A exp(-T_a/T_a) \), where \( T_a \) is the activation temperature, \( T_a = E_a/R_e, E_a \) is the activation energy and \( R_e \) is the universal gas constant \( (R_e = 1.987 \text{ [cal/g \text{- m oleK}]} \). The specific heat at

\[
\begin{align*}
1.987 \text{ [cal/g \text{- m oleK}]}.
\end{align*}
\]
constant pressure, \( c_p \), the Lewis number of the deficient reactant, \( L_e \), and the Prandtl number, \( Pr \), are all assumed to be constant. The thermal conductivity coefficient, \( \mu \), is determined from Sutherland's Law, \( \mu = \mu_0 \left( \frac{T}{T_0} \right)^{3/2} \left( \frac{T_0 + 273}{T} \right) \), where \( \mu_0 \) is a reference viscosity at temperature \( T_0 \), and \( S_l \) is a constant. The first term on the right hand side of eq. (2) is identically zero and the source terms are determined from:

\[
\frac{dY_R}{dt} = \frac{\dot{w}_R}{\rho} \tag{7}
\]

\[
\frac{dT}{dt} = -\Delta h_f \frac{\dot{w}_R}{(\rho c_p)}. \tag{8}
\]

The overall activation energy is obtained by the method suggested by Abdel-Gayed et al. (1984). Methane-air flame data was taken directly from fig. 19 of Abdel-Gayed et al. (1984) (data was from laminar flame experiments for lean to stoichiometric flames). The slope of the line \( \ln(S_L) \approx 1/2 \ln(A) - (1/T_p)(T_p/2) \) is approximately equal to one half of the activation temperature \( T_a \), and from this we determined \( T_a = 14786 \) [K], and \( E_a = 29380 \) [cal/g-mole] which is consistent with values suggested by Westbrook and Dryer (1981), Coffee et al. (1983), and Fenn et al. (1953). The product temperatures for methane-air flames, were chosen from Andrews and Bradley (1972) and the pre-exponential factor was chosen so that the laminar flame speed of the stoichiometric flame matches the experimentally determined stoichiometric flame speed. Off stoichiometric flame speeds were then determined by changing the heat release by adjusting the product temperature \( h_f = c_p(T_p - T_f) \). Here, the overall activation energy and the pre-exponential factor were held constant. This is not an optimum choice, since it requires that the product temperature be adjusted to compensate for the short-comings in the global mechanism. However, the results presented here illustrate the point that the single-step mechanism can capture the laminar flame speed and thickness reasonably well. The flame speed (using the correct \( T_p \)) is under predicted for very lean mixtures (fig. 2a). Nevertheless, \( \delta_f \) based on 99.8% of the profile agrees reasonably well with the experimental data while \( \delta_{th} \) agrees with the four-step LEM and CHEMKIN-II predictions. The laminar flame parameters used in the present study appear in Table I.

There is only one reacting species in the single-step mechanism and the reaction rate can be tabulated in terms of \( Y_R, T, \) and \( \Delta t \) (the diffusion time step). This produces a two-dimensional table for \( \Delta Y_R \) and \( \Delta T \) which are defined; \( \Delta Y_R = \int_t^{t+\Delta t} \left( \frac{\dot{w}_R}{\rho} \right) dt - Y_R \) and \( \Delta T = \int_t^{t+\Delta t} \Delta h_f \left( \frac{\dot{w}_R}{\rho c_p} \right) dt - T^a \). Values are obtained from the table using bi-linear interpolation. Using the table increases computational efficiency by nearly a factor of ten compared with solving the point problem at each point in the domain and each time step. The o.d.e. solver, DVODE (part of CHEMKIN-II), is used to generate the table at the beginning of each simulation. Typical maximum relative errors in \( \Delta Y_R \) and \( \Delta T \) are less than 0.5%.

In order to compare predictions of the turbulent flame speed with experimental data, it is necessary to determine two calibration constants. The first constant, \( C_\lambda \), appears in the event frequency parameter, eq. (5). This constant is introduced in order to scale the turbulent flame speed with the model turbulent diffusivity. A similar scale factor was introduced by McMurtry et al., (1993) to match DNS and LEM large-eddy turnover time scales so that comparisons of scalar dissipation rates from DNS and LEM could be made. The second constant, \( N_q > 1 \) reduces the effective \( Re \) by reducing the range of scales between the integral length scale and \( \eta \). It should be noted that the turbulent diffusivity, eq. (3) is not changed by \( N_q \) because in the derivation of eqs. (4) and (5), \( f(l) \) is normalized by requiring \( \int_0^\infty B_l f(l) dl = 1 \), where \( B_l \) is a constant. Therefore, a change in \( N_q \) reflects a change in \( B_l \) and \( D_T \) remains constant.

The effect of \( C_\lambda \) and \( N_q \) on the normalized event frequency parameter is shown in fig. 3a. The event frequency per unit length decreases rapidly with increasing \( N_q \) and is inversely proportional to \( C_\lambda \). The effect of \( N_q \) on the length scale distribution is shown in fig. 3b. The conditions chosen for these two plots were \( Re = 10,000, L/\eta = 1000, \nu = 1.5 \times 10^{-5} \) and represent typical values encountered in high \( Re \) flows. The effect of these two model constants on the predicted turbulent flame speed are shown in figs. 4a and 4b, respectively. These tests were conducted using the G-Equation LEM, flames G1 (Table II). In fig. 4a, nine simulations were run for values of \( u'/S_L = 5, 15, \) and 25 with \( C_\lambda = 10, 15, \) and 20. The normalized turbulent flame speeds are compared to Yakhot's model (1988) and it is apparent that a value of \( C_\lambda \) in the range of \( 10 < C_\lambda < 15 \) would closely match the present prediction with the RNG model. The constant \( C_\lambda \) causes an upward shift in the magnitude of \( u_t \) and a slightly increasing slope.
In fig. 4b \( N_\eta \) is varied for the same three \( u'/S_L \) cases as in fig. 4a. Increasing \( N_\eta \) only slightly increases the slope of the \( u'/S_L \) vs. \( u'/S_L \) curve.

The turbulent flame parameters and model constants for the simulations described in this paper are given in Table II. The turbulent flame propagation speed is determined from the time trace of the propagation of the leading flame (Kerstein, 1986). Shown in fig. 5a are time traces for various simulations each with a different \( u'/S_L \) of a lean (7% CH\(_4 \) by volume) methane-air mixture from the fan-stirred bomb experiments of Abdel-Gayed et al. (1984). These curves correspond to flames A2 in Table II. A short initial transition time is followed by a constant propagation speed which is determined by the slope of the curve. For \( u'/S_L = 1.0 \) the simulation ran for roughly 10 large-eddy turnover times and for \( u'/S_L = 25.0 \) it ran for 243 large-eddy turnover times.

In Fig. 5b the normalized turbulent flame speed predicted by the G-Equation LEM flames G1, and LEM (with finite-rate) flames A1 and A2 are compared to Yakhot's model predictions. Differences between flames A1 and A2 are the model integral length scale \( \eta \), and the number of cells required to resolve \( \eta \). LEM predictions of \( u'/S_L \) agree well with the RNG prediction for the entire range in \( u'/S_L \). Hollow symbols in fig. 5b represent individual realizations of the fan-stirred experiments and the dotted curve is the best fit to the data given by the authors (Abdel-Gayed et al. 1984). Although, the LEM predictions show differences in both magnitude and shape compared to the dotted line, they are still well within the spread of the experimental data. It was reported by the authors that the flames extinguish above \( u'/S_L = 25 \). This feature cannot be captured with the present approach since the LEM flame brush is supported from behind by a hot bath of products, while in the experiments, the flame propagation is unsteady and a significant amount of cold reactants surrounds the initial flame kernels. It may be possible to simulate extinction using the LEM with different initial conditions and boundary conditions. This issue is currently being explored.

Two other flames, A3 and A4 were also compared with experimental data from the same apparatus. These simulations were run with different values of \( S_L \) and \( N_\eta \) (see Table II) but with the same C\(_\lambda\), as in flames G1, A1, and A2. The turbulent flame speed predictions are less satisfactory than the predictions for flames G1, A1, and A2 which demonstrates that the model constants may be functions of \( S_L \), \( Le \), and/or \( \eta/\delta \). This issue is still under investigation.

Characteristics of the flame structure are examined as a function of \( u'/S_L \) in figs. 5d-5f. In fig. 5d, the radius of curvature (normalized by the experimental integral scale, \( i = 0.037 \) [m]) for three of the six A2 set of simulations is presented. As expected, the curvature decreases with increasing \( u'/S_L \). The probability of large radii of curvature decreases with increasing \( u'/S_L \) because as \( u' \) increases, the probability distribution of eddy sizes shifts to smaller eddies and therefore, the small scales are more frequently chosen for the stirring event. There is a slightly increased probability in the positive tail region for all three cases. This increased probability is due to laminar propagation and thermal expansion, both increase the radius of curvature. However, this slight increase is almost completely nullified by the high turbulence intensity at \( u'/S_L = 25 \).

In fig. 5e, the LEM flame surface density for all six simulations is presented. The flame surface density is calculated by time averaging the number of flames (defined as a scalar crossing of \( Y_R = 0.5 \)) at a location relative to the flame center. The plot has been cropped at the top to accentuate the flame structure. The spike in all six cases (which reduces as \( u'/S_L \) increases) is present because there are times when only one flame is in the domain and it will be located at the flame center so the average number of flames will be highest there. The flame surface density ranges from 2.5 to 5.0 integral scales over the range in \( u'/S_L \). The shape of the flame brush is nearly symmetric. Figure 5f is a plot of the reactant consumption rate. Its character is very representative of the flame brush. The width of the reaction zone increases with \( u'/S_L \), and its shape is nearly symmetric about the flame center.

The LEM was also compared to the weak-swirl burner flame data of Bedat and Cheng (1995), (see Table I and II, flames B1-B4). The weak-swirl burner creates a slightly diverging flow on the periphery of the outer co-flowing jet. The inner jet contains a nearly isotropic turbulent flow generated by a grid followed by a convergent nozzle upstream of the burner lip. The divergent flow stays mainly on the periphery, creating on the burner axis a decelerating flow so that a stable flame front is achieved. Four flames were investigated: two in the corrugated flamelet regime and two in the distributed combustion regime. The LEM model using the \( R \Rightarrow P \) mechanism with constant
pre-exponential factor and activation energy was cal-
ibrated for Case I with \( T_p \) obtained from Andrews
and Bradley (1972) data. The laminar flame speed
of the other three flames were determined by varying
\( T_p \) until the reported value was achieved. This re-

sults in slightly higher temperatures for the \( \phi = 0.6 \)
and \( \phi = 0.65 \) cases. The authors report for Case I tur-
bulent flow parameters and B7, B4, and
B8, corresponding to Case IV of Bedat and Cheng
(1995). The first three flames have \( S_L = 0.33 \) with
different pre-exponential factors and different activa-
tion energies, while the second set of three flames
have \( S_L = 0.15 \). The lowest activation energy, \( E_a = 9652 \text{ [cal/g — mole]} \) was extrapolated from Table I of
Abdel-Gayed \textit{et al.} (1984), using \( T_a \) and \( S_L \) from the
8.5% and 7% \( CH_4 \) flame data and the highest activa-
tion energy \( E_a = 36421 \text{ [cal/g — mole]} \) was obtained by
extrapolating in terms of % concentration using the
same data. These two extrapolation methods are
admittedly crude, compared to the method used ear-
lier (see discussion on fig. 2a and 2b). Although,
these activation energies are considered reasonable it
will be shown that this choice effects the turbulent
flame speed. The flame propagation time traces of
the simulations are shown on figs. 7a and 7b. In fig.
7a, \( u'/S_L = 1.8 \) and the traces of all three flames are
nearly the same. However, in fig. 7b, \( u'/S_L = 11.33 \)
and flame B7 has a significantly higher flame speed
than the other two flames, B4 and B8. An order of
magnitude difference in \( D_a \), 162 for the flames B5,
B1, and B6 and 12 for flames B7, B4, and B8 may
explain why the turbulent flame speed varies in this
manner for the low \( S_L \) simulations.

In fig. 8, results from simulations of four different
\( Re \) are presented. Flame B1, B4, B9, and B10 were
simulated at four different \( u' \). The normalized tur-
bulent flame speed is plotted for constant \( Re \) against
\( S_L/u' \). The data shows agreement in the general
trends seen by Abdel-Gayed \textit{et al.} (1979), at low

turbulence intensity. The curves seem to collapse as
\( S_L/u' \) increases. However, as \( u' \) increases, the LEM
flame \( u'/S_L \) reaches a plateau and as \( u' \) increases
further, \( u'/S_L \) tends toward zero. This may be the
result of turbulent diffusion. As \( S_L \) decreases, the
flame thickness generally increases so as \( S_L/u' \) de-
creases, the ratio \( \eta/\delta_t \) decreases. This would indicate
that the turbulent diffusivity is becoming more im-
portant in the flame structure. The affect of small
scale stirring may affect the propagation rate through
the redistribution of heat by the action of turbulent
diffusion, causing a reduction in the overall reaction
rates within the flame.

4 Conclusions

The structure and propagation characteristics of tur-
bulent premixed flames have been investigated using
one-dimensional simulations based on the linear-eddy model LEM (Kerstein, 1991). Extensions to an earlier LEM model were carried out to include finite-rate kinetics, thermo-diffusive, and heat release effects. LEM predictions of $u'/S_L$ are in good agreement with Yakhot's (1988) model over a wide range in $u'/S_L$. Reasonable quantitative agreement with high-Re experiments are also obtained. The rapid increase of $u'/S_L$ with increase in the normalized turbulence intensity at low $u'/S_L$ followed by the bending of the curve at higher $u'/S_L$ is reproduced. The LEM-analog of the flame surface density shows that the flame area and width of the flame brush increases with an increase in $u'/S_L$. The pdf of flame radius of curvature is nearly symmetric and the mean radius decreases with increasing $u'/S_L$. Comparisons with an earlier model based on the "G-Equation" (Menon and Kerstein 1992) show that the predictions of the propagation speeds are in good agreement.

The LEM fails to predict the turbulent flame speed of the weak-swirl burner experiments of Bedat and Cheng (1995), however, the flame brush width is predicted to within a factor of two and the pdf's of the progress variable at different locations within the flame show the onset of distributed combustion in agreement with the Borghi phase diagram. Simulations designed to evaluate the sensitivity of the activation energy demonstrate the model's capability predict propagation rate trends based on Damkohler number.

Trends in $u'/S_L$ based on $S_L/u'$ for different Re are also captured by the model. The normalized turbulent flame speed decreases with increasing $S_L/u'$ in agreement with experimental data by Abdel-Gayed et al. (1979), but at low $S_L/u'$ (high $u'$) the LEM predicts a plateau in $u'/S_L$.

These results demonstrate that the LEM approach can capture many underlying features of the premixed flame and is capable of predicting the turbulent flame speed. The demonstration that the LEM can be used to study high Reynolds number premixed flames may make this simulation model a valuable tool for analysing turbulent premixed flames. Further work is needed to describe the functional form of model constants.

Acknowledgments

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References


Table I. Laminar Flame Properties.

<table>
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<tr>
<th>Flame</th>
<th>$S_L$ [m/sec.]</th>
<th>$\delta_{4b} \times 10^4$ [m]</th>
<th>$\nu \times 10^8$ [m$^2$/sec.]</th>
<th>$Le$</th>
<th>$A$ [sec.$^{-1}$]</th>
<th>$E_a$ [cal/g - mol]</th>
<th>$T_f$ [K]</th>
<th>$T_p$ [K]</th>
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<td>0.36</td>
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<td>39422</td>
<td>328</td>
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Table II. Turbulent Flame Properties.

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Fig. 1a. Schematic diagram of the LEM simulation domain. Flame brush, flame center and radius of curvature are also defined.

Fig. 1b. Snapshot of the flame brush in terms of normalized mass fraction for $u'/S_L=30$.

Fig. 2a. Laminar flame speed as a function of equivalence ratio for methane–air mixtures.

Fig. 2b. Laminar flame thickness as a function of equivalence ratio for methane–air mixtures.
Fig. 3a. Normalized stirring rate parameter for different stirring rate constants, $C_\lambda$, as a function of $N_\eta$.

Fig. 3b. Distribution function of eddy sizes chosen for stirring events.

Fig. 4a. Normalized turbulent flame speed as a function of normalized turbulence intensity, predicted by G–LEM, for different stirring rate constants, $C_\lambda$.

Fig. 4b. Normalized turbulent flame speed as a function of normalized turbulence intensity, predicted by G–LEM for different model constants, $N_\eta$.

Fig. 5a. Time trace of flame front propagation of flames A2 for different $u'/S_L$.

Fig. 5b. Normalized turbulent flame speed for flames G1, A1, and A2, compared with Yakhot's model, (1988), and fan–stirred bomb experiments of Abdel–Gayed et al., (1984).
Fig. 5c. Normalized turbulent flame speed, for flames A3 and A4, compared with Yakhot's (1988), model and fan-stirred bomb experiments of Andrews et al., (1974), and Abdel-Gayed et al., (1984).

Fig. 5e. LEM flame surface density of flames A2, for different \( u'/S_L \).

Fig. 5d. Probability density of radius of curvature of flames A2, for different \( u'/S_L \).

Fig. 5f. Mean mass reactant consumption rate of flames A2, for different \( u'/S_L \).

Fig. 6a. Mean and variance of the progress variable \( \langle C \rangle \) for flames B1 and B4.

Fig. 6b Probability density at different locations in the flame represented by \( \langle C \rangle \) for flame B1, corresponding to Case I of Bedat and Cheng (1995).
Fig. 6c. Probability density at different locations in the flame represented by $<C>$ for flame B4, corresponding to Case 4 of Bedat and Cheng (1995).

Fig. 7a. Time trace of flame front propagation for flames B5, B1, and B6 with $u'/S_L=1.8$ and $S_L=0.30$, for different activation energies.

Fig. 7b. Time trace of flame front propagation for flames B7, B4, and B8 with $u'/S_L=11.3$ and $S_L=0.15$, for different activation energies.

Fig. 8. Normalized turbulent flame speed as a function of normalized laminar flame speed for flames B1, B4, B9, and B10, for different Re compared with fan-stirred bomb experiments of Abdel-Gayed et al., (1979).