Research Article

**A Priori** Assessment of Algebraic Flame Surface Density Models in the Context of Large Eddy Simulation for Nonunity Lewis Number Flames in the Thin Reaction Zones Regime

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The performance of algebraic flame surface density (FSD) models has been assessed for flames with nonunity Lewis number (Le) in the thin reaction zones regime, using a direct numerical simulation (DNS) database of freely propagating turbulent premixed flames with Le ranging from 0.34 to 1.2. The focus is on algebraic FSD models based on a power-law approach, and the effects of Lewis number on the fractal dimension $D$ and inner cut-off scale $\eta_i$ have been studied in detail. It has been found that $D$ is strongly affected by Lewis number and increases significantly with decreasing Le. By contrast, $\eta_i$ remains close to the laminar flame thermal thickness for all values of Le considered here. A parameterisation of $D$ is proposed such that the effects of Lewis number are explicitly accounted for. The new parameterisation is used to propose a new algebraic model for FSD. The performance of the new model is assessed with respect to results for the generalised FSD obtained from explicitly LES-filtered DNS data. It has been found that the performance of the most existing models deteriorates with decreasing Lewis number, while the newly proposed model is found to perform as well or better than the most existing algebraic models for FSD.

1. Introduction

Reaction rate closure based on flame surface density (FSD) is one of the most popular approaches to combustion modelling in turbulent premixed flames [1–11]. In the context of LES the generalised FSD ($\Sigma_{gen}$) is defined as follows [3–11]:

$$\Sigma_{gen} = |\nabla c|.$$  \hspace{1cm} (1)

where the overbar denotes the LES filtering operation. The reaction progress variable $c$ may be defined in terms of a reactant mass fraction $Y_R$, for example, $c = (Y_{R0} - Y_R)/(Y_{R0} - Y_{R\infty})$ such that $c$ rises monotonically from zero in fresh reactants (subscript 0) to unity in fully burned products (subscript $\infty$).

In the context of LES, several models have been proposed for the wrinkling factor $\Xi$ [12–16], which is often used in the context of thickened flame modelling [13, 14]. The wrinkling factor $\Xi$ is closely related to $\Sigma_{gen}$ according to [12–16]:

$$\Xi = \frac{\Sigma_{gen}}{|\nabla \tau|}. \hspace{1cm} (2a)$$

Often, $\Xi$ is expressed in terms of a power-law expression [7, 9, 13, 14] $\Xi = (\eta_0/\eta_i)^{D-2}$ in which $\eta_0$ and $\eta_i$ are the outer and inner cut-off scales and $D$ is the fractal dimension. This leads to a power-law expression for $\Sigma_{gen}$ as:

$$\Sigma_{gen} = \Xi |\nabla \tau| = \left(\frac{\Delta}{\eta_i}\right)^{D-2} |\nabla \tau|, \hspace{1cm} (2b)$$

where $\Delta$ is the grid size.
where, for LES, the outer cut-off scale $\eta_{ig}$ is taken to be equal to the filter width $\Delta$. According to Peters [17], $\eta$ scales with the Gibson length scale $L_G = S_f/\kappa$ in the corrugated flamelets (CF) regime, and with the Kolmogorov length scale $\eta = (\nu^3/\varepsilon)^{1/4}$ in the thin reaction zones (TRZ) regime. Here, $S_f$ is the unstrained laminar burning velocity, $\nu$ is the kinematic viscosity in the unburned gas, and $\varepsilon$ is the dissipation rate of turbulent kinetic energy. Experimental analyses by Knikker et al. [7] and Roberts et al. [18] indicated that $\eta$ scales with the Zel’dovich flame thickness $\delta_Z = a_{f0}/S_f$, where $a_{f0}$ is the thermal diffusivity in unburned gases. A recent a priori DNS analysis [9] demonstrated that $\eta$ scales with $L_G$ and $\eta$ for the CF and TRZ regimes, respectively, as suggested by Peters [17]. However, $\eta$ is also found to scale with thermal flame thickness $\delta_Z$ in both the CF and TRZ regimes [9].

North and Santavicca [19] parameterised $D$ in terms of the root-mean-square (rms) turbulent velocity fluctuation $u’$ as: $D = 2.65/\langle u’ \rangle^2 + 1.25/\langle S_f / u’ \rangle + 1$, whereas Kerstein [20] suggested that $D$ increases from 2 to 7/3 for increasing values of $u’/S_f$, where $D = 7/3$ is associated with the material surface.

Since combustion is set to remain a major practical means of energy conversion for the foreseeable future, it has become necessary to find novel ways to reduce carbon emissions from relatively conventional combustion systems. One such approach is the use of hydrogen-blended hydrocarbon fuels in IC engines, aeroengines, and furnaces. Increased abundance of fast diffusing species such as H and $H_2$ leads to significant effects of differential diffusion of heat and mass in hydrogen-blended flames [21, 22], whereas these effects are relatively weaker in conventional hydrocarbon flames [22, 23]. The differential rates of thermal and mass diffusion in premixed flames are often characterised by the Lewis number $Le$ which is defined as the ratio of the thermal diffusivity to mass diffusivity (i.e., $Le = \alpha_l/D_c$). Assigning a local characteristic value of $Le$ is not straightforward since many species with different individual values of $Le$ are involved in actual combustion. Often the Lewis number of the deficient reactant species is used as the characteristic $Le$ [21, 24–28] and this approach has been adopted here. It is worth noting that, to date, most FSD-based modelling has been carried out for unity Lewis number flames (e.g., [1–11]) and the effects of differential diffusion of heat and mass on the statistical behaviour of FSD have rarely been addressed [28]. More specifically the effects of $Le$ on $D$ and $\eta_l$ have not yet been analysed in detail, or in the context of power-law FSD reaction rate models. Moreover, most algebraic models for $\Sigma_{gen}$ have been proposed for the CF regime where the effects of $Le$ are not accounted for. Thus, it is important to assess the performance of existing models for combustion in the TRZ regime with nonunity Lewis number.

The present study aims to bridge this gap in the existing literature. In this respect the main objectives of the work are as the following.

(i) To understand the effects of Lewis number on $D$ and $\eta_l$, in the context of LES modelling.

(ii) To assess the performance of existing wrinkling factor-based algebraic models of FSD in the context of LES for flames with nonunity global Lewis number based on a priori DNS analysis.

(iii) To identify or develop a power-law-based algebraic model for FSD in the context of LES which is capable of predicting the correct behaviour of FSD even for nonunity Lewis number flames.

The rest of the paper is organised as follows. An overview of the different algebraic FSD models considered here are presented in the next section. This will be followed by a brief discussion of the numerical implementation. Following this, results will be presented and subsequently discussed. Finally the main findings will be summarised and conclusions will be drawn.

2. Overview of Power-Law-Based FSD Models

A model for $\Sigma$ suggested by Angelberger et al. [4] (FSDA model) can be written in terms of $\Sigma_{gen}$ as follows:

$$\Sigma_{gen} = \left[1 + a\Gamma \left(\frac{u_A}{\langle S_f \rangle}\right) \right] \nabla \tau|_{\kappa},$$

where $a = 1$ is a model parameter, $u_A = \sqrt{2\kappa_\delta / 3}$ is the subgrid turbulent velocity fluctuation, $k_\delta = (\langle \ddot{u}_i \ddot{u}_j \rangle / \langle u_i u_j \rangle / 2)$ is the subgrid turbulent kinetic energy and $Q = \rho Q_{gen}$ denotes the Favre-filtered value of a general quantity $Q$. In (3a), $\Gamma$ is an efficiency function which is given by:

$$\Gamma = 0.75 \exp \left[-1.2 \left(\frac{u_A}{\langle S_f \rangle}\right)^{-0.3} \left(\frac{\Delta}{\delta_\zeta}\right)^{2/3}\right].$$

Weller et al. [12] also presented an algebraic model for $\Sigma$, which can be recast in the form (FSDW model):

$$\Sigma_{gen} = [1 + 2(\Theta - 1)] \nabla \tau|_{\kappa},$$

where $\Theta = 1 + 0.62 (\langle u_A \rangle / \langle S_f \rangle) Re_c$ and $Re_c = u_A \cdot \rho \eta / \mu_0$ with $\eta$ and $\mu_0$ denoting the Kolmogorov length scale and unburned gas density respectively. Colin et al. [13] proposed an algebraic model for $\Sigma$, which can be expressed in terms of FSD (FSDC model) as:

$$\Sigma_{gen} = \left[1 + a \Gamma \left(\frac{u_A}{\langle S_f \rangle}\right) \right] \nabla \tau|_{\kappa},$$

where $a = b = 1$ and $\eta_l$ have been taken into account, or in the context of power-law FSD reaction rate models. Moreover, most algebraic models for $\Sigma_{gen}$ have been proposed for the CF regime where the effects of $Le$ are not accounted for. Thus, it is important to assess the performance of existing models for combustion in the TRZ regime with nonunity Lewis number.

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$$\Sigma_{gen} = \left[1 + a \Gamma \left(\frac{u_A}{\langle S_f \rangle}\right) \right] \nabla \tau|_{\kappa},$$

where $\Gamma$ is given by (3b), $a = b = 1$, $\alpha_l = \beta \times 2 \ln(2)/[3c_{ms}(Re_{c/2} - 1)]$ with $Re_{c/2} = \rho_0 u_\infty / \mu_0$, where $\mu_0$ is the unburned gas viscosity and $l$ is the integral length scale, $\beta = 1.0$ and $c_{ms} = 0.28$. The FSDC model requires three input parameters, namely $u_A/\langle S_f \rangle$, $\alpha_l/\delta_\zeta$, and $Re_c$. Charlette et al. [14] reduced the input parameters to only $u_A/\langle S_f \rangle$ and $\alpha_l/\delta_\zeta$ by using (FSDCH model):

$$\Sigma_{gen} = \left[1 + \min \left(\frac{\Delta}{\delta_\zeta}, \Gamma_\Delta \left(\frac{u_A}{\langle S_f \rangle}\right)\right) \right] \nabla \tau|_{\kappa},$$

with the efficiency function

$$\Gamma_\Delta = \left[\left(\frac{f\sigma}{a} + f_\Delta^{\alpha_l}\right)^{-1/\alpha_l} \right]^{-1/a_l} + f^{h_\Delta} \cdot \left(f_\Delta^{h_\Delta} \right)^{-1/b},$$
where \( \Re_\Delta = u' \Delta / v \) and with model constants \( b_1 = 1.4, \beta_1 = 0.5, C_k = 1.5 \), and functions \( a_1, f_u, f_\Sigma \), and \( f_{\Re_\Delta} \) are defined by:

\[
\begin{align*}
    a_1 &= 0.60 + 0.20 \exp[-0.1 \frac{u'_s}{S_L}] - 0.20 \exp[-0.01 \frac{\Delta}{\delta_c}], \\
    f_u &= 4 \left( \frac{27}{110} C_k \right)^{1/2} \left( \frac{u'_s}{S_L} \right)^2, \\
    f_\Sigma &= \frac{27}{55} C_k \pi^{4/3} \left( \frac{\Delta}{\delta_c} \right)^{4/3} - 1 \right]^{1/2}, \\
    f_{\Re_\Delta} &= \left[ \frac{9}{55} \exp(-1.5 C_k \pi^{4/3} \Re_\Delta^{-1}) \right]^{1/2} \Re_\Delta^{1/2}.
\end{align*}
\] (7b)

Knikker et al. [7] proposed a model for \( \Sigma_{gen} \) (FSDF model) as:

\[
\Sigma_{gen} = \left( \frac{\Delta}{\eta_l} \right)^{\beta_k} |\nabla \tilde{v}|, \tag{8}
\]

where the inner cut-off scale \( \eta_l \) is taken to be \( \eta_l = 3 \delta_c \) and \( \beta_k \) is estimated based on a dynamic formulation as \( \beta_k = [\log(|\nabla \tilde{v}|) - \log(|\nabla \tilde{\eta}|)] / \log \gamma \), where \( \tilde{v} \) denotes the reaction progress variable at the test filter level \( \gamma \Delta \). Fureby [16] proposed a model for \( \Sigma \) which can be written in terms of \( \Sigma_{gen} \) (FSDF model) as:

\[
\Sigma_{gen} = \left[ \Gamma \left( \frac{u'_s}{S_L} \right) \right]^{D-2} \cdot |\nabla \tau|, \tag{9}
\]

where \( \Gamma \) is given by (3b), and \( D \) is specified according to the parameterisation \( D = 2.05/(u'_s/S_L + 1) + 2.35/(S_L/u'_s + 1) \) [19].

In the present study, the performance of each algebraic model described above is assessed with respect to \( \Sigma_{gen} \) obtained from DNS. There are three requirements for each model. Firstly, the volume-averaged value of \( \Sigma_{gen} \) represents the total flame surface area, and therefore this quantity should not change with \( \Delta \). Secondly, the model should be able to capture the correct variation of the averaged value of \( \Sigma_{gen} \) conditional on \( \tau \) across the flame brush. Thirdly, the correlation coefficient between the modelled and actual values of \( \Sigma_{gen} \) should be as close to unity as possible in order to capture the effects of local strain rate and curvature on \( \Sigma_{gen} \).

### 3. Numerical Implementation

For the purposes of the analysis, a DNS database of three-dimensional turbulent premixed flames has been generated using the compressible DNS code SENGa [29]. Until recently most combustion DNS was carried out either in three dimensions with simplified chemistry or in two dimensions with detailed chemistry due to the limitations of available computational power. Although it is now possible to carry out three-dimensional DNS with detailed chemistry, such computations remain extremely expensive [30] and are not practical for a parametric study as in the present case. Thus three-dimensional DNS with single-step Arrhenius type chemistry has been used in the present study in which the effects of Lewis number are to be investigated in isolation.

For the present DNS database, the computational domain is considered to be a cube of size \( 24.1 \delta_b \times 24.1 \delta_b \times 24.1 \delta_b \), which is discretised using a uniform grid of \( 230 \times 230 \times 230 \). The grid spacing is determined by the flame resolution, and in all cases, about 10 grid points are kept within \( \delta_b = (T_{ad} - T_b) / \max |\nabla T|_l \), where \( T_{ad} \) and \( T_b \) are the adiabatic flame, unburnt reactant and instantaneous dimensional temperatures respectively, and the subscript \( L \) is used to refer to unstrained planar laminar flame quantities. The boundaries in the direction of mean flame propagation are taken to be partially nonreflecting and are specified using the Navier Stokes Characteristic Boundary Conditions formulation [31], while boundaries in the transverse direction were taken to be periodic. A 10th order

**Table 1**

(a) Initial values of the simulation parameters and nondimensional numbers relevant to DNS database

<table>
<thead>
<tr>
<th>Case</th>
<th>Le</th>
<th>( u'/S_L )</th>
<th>( l/\delta_b )</th>
<th>( \tau )</th>
<th>( \Re )</th>
<th>( Da )</th>
<th>( \Da )</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>0.34</td>
<td>7.5</td>
<td>2.45</td>
<td>4.5</td>
<td>47.0</td>
<td>0.33</td>
<td>9.92</td>
</tr>
<tr>
<td>B</td>
<td>0.6</td>
<td>7.5</td>
<td>2.45</td>
<td>4.5</td>
<td>47.0</td>
<td>0.33</td>
<td>9.92</td>
</tr>
<tr>
<td>C</td>
<td>0.8</td>
<td>7.5</td>
<td>2.45</td>
<td>4.5</td>
<td>47.0</td>
<td>0.33</td>
<td>9.92</td>
</tr>
<tr>
<td>D</td>
<td>1.0</td>
<td>7.5</td>
<td>2.45</td>
<td>4.5</td>
<td>47.0</td>
<td>0.33</td>
<td>9.92</td>
</tr>
<tr>
<td>E</td>
<td>1.2</td>
<td>7.5</td>
<td>2.45</td>
<td>4.5</td>
<td>47.0</td>
<td>0.33</td>
<td>9.92</td>
</tr>
</tbody>
</table>

(b) List of initial simulation parameters and nondimensional numbers for the DNS database based on which the \( \Re \) dependence of \( D \) is parameterised

<table>
<thead>
<tr>
<th>Case</th>
<th>( u'/S_L )</th>
<th>( l/\delta_b )</th>
<th>( \tau )</th>
<th>( \Re )</th>
<th>( Da )</th>
<th>( \Da )</th>
</tr>
</thead>
<tbody>
<tr>
<td>A1</td>
<td>5.0</td>
<td>1.67</td>
<td>4.5</td>
<td>22</td>
<td>0.33</td>
<td>6.54</td>
</tr>
<tr>
<td>B1</td>
<td>6.25</td>
<td>1.44</td>
<td>4.5</td>
<td>23.5</td>
<td>0.23</td>
<td>9.84</td>
</tr>
<tr>
<td>C1</td>
<td>7.5</td>
<td>2.5</td>
<td>4.5</td>
<td>49.0</td>
<td>0.33</td>
<td>9.84</td>
</tr>
<tr>
<td>D1</td>
<td>9.0</td>
<td>4.31</td>
<td>4.5</td>
<td>100.0</td>
<td>0.48</td>
<td>9.84</td>
</tr>
<tr>
<td>E1</td>
<td>11.25</td>
<td>3.75</td>
<td>4.5</td>
<td>110</td>
<td>0.33</td>
<td>14.73</td>
</tr>
</tbody>
</table>
central difference scheme was used for spatial discretisation for internal grid points and the order of differentiation gradually decreases to a one-sided second-order scheme at non-periodic boundaries [29]. A low storage 3rd-order Runge-Kutta scheme [32] is used for time advancement. The turbulent velocity field is initialised by using a standard pseudo-spectral method [33], and the flame is initialised using an unstrained planar steady laminar flame solution.

The initial values of \( u'/S_L \) and \( l/\delta_{bh} \) for all the flames considered here are shown in Table 1 along with the values of heat release parameter \( \tau = (T_{ad} - T_0)/T_0 \), Damköhler number \( Da = lS_L/u' \delta_{bh} \), Karlovitz number \( Ka = (u'/S_L)^{1/2}(lS_L/\alpha_{T0})^{-1/2} \) and turbulent Reynolds number \( Re_t = \rho_0 u'/\mu_0 \). For all cases \( Ka \) remains greater than unity, which indicates that combustion is taking place in the TRZ regime [17]. Standard values are taken for Prandtl number \( (Pr = 0.7) \), ratio of specific heats \( (\gamma_G = C_p/C_v = 1.4) \), and the Zel’dovich number \( (\rho Z = T_{ad}/T_0) \) for internal grid points and the order of differentiation. By contrast, the quantity \( (\nabla \tau) \) denotes the resolved portion of the flame wrinkling, which decreases with increasing \( Da \). As a result, \( \log([\Sigma_{gen}]/(\nabla \tau)) \) increases with increasing \( Da \). The variation of \( \log([\Sigma_{gen}]/(\nabla \tau)) \) with \( \log(\Delta/\delta_t) \) is linear when \( \Delta \gg \delta_t \) but becomes nonlinear for \( \Delta \ll \delta_t \). The best-fit straight line representing the greatest slope of the linear variation has been used to obtain values of \( D \) and \( \eta_i \). It has been found that \( \eta_i/\delta_t \) remains independent of \( Le \), and for all cases \( \eta_i \) remains on the order of thermal flame thickness \( \delta_{th} \) (i.e., \( \eta_i/\delta_{th} = 1.0 \)), which is about twice the Zel’dovich flame thickness \( \delta_z \) for the present thermochemistry (i.e., \( \eta_i = 1.796 \delta_z = \delta_{th} \)). The scaling of the inner cut-off scale \( \eta_i \) with \( \delta_z \) is consistent with previous DNS [9] and experimental [7, 18] findings. Figure 1 shows that the slope of the linear region decreases with increasing Lewis number (i.e., in moving from case a to case e), which suggests that the fractal dimension \( D \) decreases with increasing \( Le \).

4. Results and Discussion

4.1. Effects of \( Le \) on \( D \) and \( \eta_i \). The power law expression (2b) for \( \Sigma_{gen} \) may be rewritten as:

\[
\log \left( \frac{\langle \Sigma_{gen} \rangle}{\langle \nabla \tau \rangle} \right) = (D - 2) \log \Delta - (D - 2) \log(\eta_i) \tag{10}
\]

where the angled brackets indicate a volume-averaging operation. The variation of \( \log([\Sigma_{gen}]/(\nabla \tau)) \) with the ratio \( (\Delta/\delta_t) \) is shown in Figure 1 on a log-log plot for all the different Lewis number cases. The quantity \( \langle \Sigma_{gen} \rangle \) denotes the total flame surface area which remains independent of filter size \( \Delta \). However, these regime diagrams have been proposed based on scaling arguments for unity Lewis number flames and the likely effects of nonunity Lewis number on these regime diagrams have yet to be ascertained. This topic is the subject of a separate investigation and will not be taken up in this paper.

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\]
Figure 1: Variation of $\langle \Sigma_{gen} \rangle / \langle \nabla \tau \rangle$ with $\Delta/\delta_z$ on a log-log plot for (a–e) cases A–E. Prediction of $(\Sigma_{gen})/\langle \nabla \tau \rangle = (\Delta/\eta_i)^{D-2}$ with $\eta_i$ obtained from DNS and $(D - 2)$ according to (11) is also shown.
global Lewis number (i.e., $Ka$, $Re$, and $Le$) according to the following:

\[ D = 2 + \frac{1}{3} \text{erf}(3.0 Ka) \left[ 1 - \exp \left( -0.1 \left( \frac{Re}{A_m} \right)^{1.6} \right) \right] \text{Le}^{-0.45}, \]

where $A_m \approx 7.5$ is a model parameter. Further details on the basis of this parameterisation are given in Appendix A.

The prediction of $(\Sigma_{gen})/(\gamma |\nabla c|) = (\Delta/\eta_i)^{D-2}$ with $\eta_i$ obtained from DNS and $D$ obtained from (11) is also shown in Figure 1, which indicates that (11) satisfactorily captures the best-fit straight line corresponding to the

Figure 2: Contours of $c$ in the $x_1 - x_2$ midplane at time $t = \delta_{th}/S_L$ for (a–e) cases A–E.
power law. It is worth noting that $Re_t$ and $Ka$ in (11) were evaluated for this purpose based on $u'/\lambda$ and $l/\delta_h$ in the unburned reactants. However, in actual LES simulations, $D$ needs to be evaluated based on local velocity and length scale ratios (i.e. $u'_\Delta/\lambda$ and $\Delta/\delta_h$). Here $u'_\Delta$ is estimated from the subgrid turbulent kinetic energy as $u'_\Delta = \sqrt{\frac{2\epsilon}{3}}$ following previous studies [12, 15, 16]. The local Karlovitz number $Ka_\Delta$ can be evaluated as $Ka_\Delta = C_{ka}(\sqrt{\epsilon/\lambda})^{3/2}(\delta_h/\Delta)^{1/2}$, where $C_{ka}$ is a model parameter. Similarly, the local turbulent Reynolds number $Re_\Delta$ can be evaluated using $Re_\Delta = C_{Re}(\rho u'_\Delta \Delta/\mu_0)$. The choice of model constants $C_{ka} = 6.6$ and $C_{Re} = 4.0$ ensures an accurate prediction of $D$ for $\Delta \gtrsim \eta$, and yields the value of $D$ obtained based on the global quantities according to (11).

Figure 3: Percentage error (13) of the model prediction from $\langle \Sigma_{gen} \rangle$ obtained from DNS for LES filter widths $\Delta = 4\Delta_m = 0.4\delta_h$; $\Delta = 8\Delta_m = 0.8\delta_h$; $\Delta = 12\Delta_m = 1.2\delta_h$; $\Delta = 16\Delta_m = 1.6\delta_h$; $\Delta = 20\Delta_m = 2.0\delta_h$; $\Delta = 24\Delta_m = 2.4\delta_h$ for (a–e) cases A–E.

Based on the observed behaviour of $D$ and $\eta$, a power-law expression for $\Sigma_{gen}$ is proposed here (model FSDNEW):

$$\Sigma_{gen} = |\nabla \tau| \left[ (1 - f) + f \left( \frac{\Delta}{\eta} \right)^{D-2} \right],$$

(12)

where $f$ is a bridging function which increases monotonically from zero for small $\Delta$ (i.e., $\Delta/\delta_h \to 0 \ or \ \Delta \ll \delta_h$) to unity for large $\Delta$ (i.e., $\Delta \gg \eta \ or \ \Delta \gg \delta_h$). Equation (12) ensures that $\Sigma_{gen}$ approaches $|\nabla \tau|/(\Delta/\eta)^{D-2}$ for large $\Delta$ and at the same time $\Sigma_{gen}$ approaches $|\nabla \tau|$ (i.e., $\lim_{\Delta \to \delta_h} \Sigma_{gen} = \lim_{\Delta \to \eta} |\nabla \tau| = |\nabla \tau|$) for small $\Delta$. It has been found that $\Sigma_{gen} \approx |\nabla \tau|$ provides better agreement with $\Sigma_{gen}$ obtained from DNS data for $\Delta \leq 0.8\delta_h$, whereas the power-law $\Sigma_{gen} = |\nabla \tau|/(\Delta/\eta)^{D-2}$ starts to predict $\Sigma_{gen}$ more accurately for
Figure 4: Variation of mean values of $\Sigma_{\text{gen}} \times \delta_{z}$ conditional on $\tau$ across the flame brush for $\Delta = 8\Delta_{m} = 0.8\delta_{th}$ according to DNS, FSDA, FSDC, FSDW, FSDCH, FSDK, FSDF, FSDNEW, and MFSDF predictions for (a–e) cases A–E.
Figure 5: Variation of mean values of $\Sigma_{gen} \times \delta_z$ conditional on $\tau$ across the flame brush for $\Delta = 24\Delta_m = 2.4\delta_{th}$ according to DNS, FSDA, FSDC, FSDW, FSDCH, FSDK, FSDF, FSDNEW, and MFSDF predictions for (a–e) cases A–E.
Figure 6: Variation of percentage error (17) on $\tau$ across the flame brush for $\Delta = 8\Delta_{m} = 0.8\delta_{th}$ according to FSDA, FSDC, FSDW, FSDCH, FSDK, FSDF, FSDNEW, and MFSDF predictions for (a–e) cases A–E.
Figure 7: Variation of percentage error (17) on τ across the flame brush for Δ = 24Δm = 2.4δm according to FSDA, FSDC, FSDW, FSDCH, FSDK, FSDF, FSDNEW, and MFSDF predictions for (a–e) cases A–E.
\[ \Delta \geq 1.2 \eta_i \] (see Figure 1). Based on this observation, the bridging function \( f \) is taken to be \( f = 1/[1+\exp\{-60(\Delta/\eta_i-1.0)\}] \), which ensures a smooth transition between \( 0.8 \eta_i < \Delta < 1.2 \eta_i \). As \( \eta_i \) is found to scale with \( \delta_z \) (i.e., \( \eta_i \approx 1.79 \delta_z \approx \delta_{th} \) according to the present thermochemistry), \( \eta_i \) in (12) is taken to be the thermal flame thickness \( \delta_{th} \).

The performance of the various algebraic models for \( \Sigma_{gen} \) will be assessed next, using the model requirements stated earlier.

### 4.2. Performance of Models for the Volume-Averaged FSD (\( \langle \Sigma_{gen} \rangle \))

The inaccuracy in the model predictions of \( \langle \Sigma_{gen} \rangle \) can be characterised using a percentage error (PE):

\[
PE = \frac{\langle \Sigma_{gen}\rangle_{\text{model}} - \langle \Sigma_{gen}\rangle}{\langle \Sigma_{gen}\rangle} \times 100, \tag{13}
\]

where \( \langle \Sigma_{gen}\rangle_{\text{model}} \) is the volume-averaged value of the model prediction of \( \langle \Sigma_{gen}\rangle \). Results for the PE for a range of filter size \( \Delta \) are shown Figure 3. These demonstrate that the models denoted by FSDA (see (3a) and (3b)) and FSDC (see (5)) overpredict \( \langle \Sigma_{gen}\rangle \) for all the Lewis number cases, and that the level of overprediction increases with increasing \( \Delta \). The FSDW model (see (4)) also overpredicts \( \langle \Sigma_{gen}\rangle \), although the level of overprediction decreases for \( \Delta \gg \delta_{th} \), especially for cases with \( \text{Le} \geq 0.6 \) (i.e., cases B–E). The FSDC model has greater PE than both the FSDA and FSDW models for all \( \Delta \) in the same cases. However, the FSDW model has the highest PE relative to both the FSDA and FSDC models for all \( \Delta \) in the \( \text{Le} = 0.34 \) case.

The FSDCH (6), FSDA, and FSDC models provide accurate predictions of \( \langle \Sigma_{gen}\rangle \) at small values of \( \Delta \) (i.e., \( \Delta \ll \delta_z \)) but they overpredict \( \langle \Sigma_{gen}\rangle \) for large values of \( \Delta \) (i.e.,
Figure 9: Variation of \( \langle \Sigma_{gen} \rangle / (\nabla |v|) \) with \( \Delta/\delta_z \) on a log-log plot for (a–e) cases A1–E1. The prediction of \( \langle \Sigma_{gen} \rangle / (\nabla |v|) = (\Delta/\eta_i)^{D-2} \) with \( \eta_i \) obtained from DNS and \( (D - 2) \) according to (11) is also shown.
\[ \Delta \gg \delta_i \). The FSDF model (9) predicts accurately for small \( \Delta \), and marginally underpredicts for larger \( \Delta \), for cases with \( \text{Le} \approx 0.6 \). However, the FSDF model remains better than the FSDA, FSDC, FSDCH, and FSDW models. The FSDNEW model (12) provides an accurate prediction of \( \Sigma_{\text{gen}} \) for all filter sizes because this model is designed to do so for all values of \( \text{Le} \). The PE for the FSCH model remains small for cases with \( \text{Le} \approx 1.0 \) (i.e., cases C–E), although the FSDCH model overpredicts \( \Sigma_{\text{gen}} \) for \( \Delta > \delta_{\text{th}} \) for cases with \( \text{Le} \ll 1 \) (i.e., cases A and B). The FSDK model (see (8)) underpredicts the value of \( \Sigma_{\text{gen}} \) for all \( \Delta \) for all cases. However, the level of underprediction of the FSDK model decreases for larger \( \Delta \).

The PEs for the FSDF and FSDNEW models remain negligible in comparison to the PEs for all the other models. Note that \( \Sigma_{\text{gen}} \) should approach \( |\nabla \tau| \) (i.e., \( \lim_{u_\Delta \to 0} \Sigma_{\text{gen}} = \lim_{u_\Delta \to 0} |\nabla \tau| \) ) when \( u_\Delta \) vanishes because the flow tends to be fully resolved (i.e., \( \lim_{\Delta \to 0} u_\Delta = 0 \) and \( \lim_{u_\Delta \to 0} \Sigma_{\text{gen}} = |\nabla \tau| \) ). Although the FSDF model performs well for all \( \Delta \) for all the cases considered here, \( \Sigma_{\text{gen}} \) does not tend to \( |\nabla \tau| \) as \( u_\Delta \) approaches zero, but instead predicts a finite value close to zero. This limitation of the FSDK model can be avoided using a modified form of (8) (MSFDF model):

\[
\Sigma_{\text{gen}} = |\nabla \tau| \left( 1 - f \right) + f \left( \Gamma \cdot \nabla \right)^{D-2},
\]

where \( f = 1 / [1 + \exp(-60(\Delta/\delta_0 - 1.0))] \) is a bridging function as before, the efficiency function \( \Gamma \) is given by \( (3b) \) and \( D = 2.05/(u_{\text{th}}/S_1 + 1) + 2.35/(S_1/u_{\text{th}} + 1) \) [19]. Equation (14) ensures that \( \Sigma_{\text{gen}} \) becomes exactly equal to \( |\nabla \tau| \) when the flow is fully resolved (i.e., \( \Delta \ll \eta_i \) or \( \Delta \to 0 \) ), where \( u_\Delta \) also vanishes (i.e., \( \lim_{\Delta \to 0} u_\Delta = 0 \)). Figure 3 shows that the modification given by (14) does not appreciably alter the performance of (8) while ensuring the correct asymptotic behaviour. Note that the parameterisation of \( D \) and \( \Gamma \) according to \([19] \) and \( (3b) \), respectively, is essential for the satisfactory performance of the FSDF model. Using (13), for \( D \) in the FSDK model is found to lead to a deterioration in its performance. Similarly, using \( D \) as given by [19] in (12) worsens the performance of the FSDKNEW model.

The FSDK model is based on the power-law \( \Sigma = (\eta_i/\eta)D-2 \) which is strictly valid only for filter sizes \( \Delta \) which are sufficiently greater than \( \eta_i \) (i.e., \( \Delta \gg \eta_i \)), as can be seen from Figure 1. Hence, the predictive capability of the FSDK model improves when \( \Delta > \eta_i \) (see Figure 3). However, the FSDK model underpredicts \( \Sigma_{\text{gen}} \) because the inner cut-off scale is taken to be \( 3\delta_i \) in this model whereas \( \eta_i \approx 1.79\delta_i \) for all the cases considered here. An accurate estimation of \( \eta_i \) in the framework of the FSDK model results in comparable performance to the FSDKNEW model for large \( \Delta \) (i.e., \( \Delta \gg \eta_i \)). Moreover, \( \Sigma_{\text{gen}} \) vanishes when \( \Delta \to 0 \) according to the FSDK model, whereas \( \Sigma_{\text{gen}} \) should approach \( |\nabla \tau| \) when \( \Delta \to 0 \) (i.e., \( \lim_{\Delta \to 0} \Sigma_{\text{gen}} = \lim_{\Delta \to 0} |\nabla \tau| = |\nabla \tau| \) ). This limitation can be avoided by modifying the FSDK model in the same manner as shown in (14) for the FSDK model (not shown here for conciseness).

The stretch-rate \( K = (1/\delta A)d(\delta A)/dt = \alpha_x + S_2 \nabla \cdot \vec{N} \) represents the fractional rate of change of flame surface area \( A \) [1], where \( S_d = \frac{Dc}{Dt}/|\nabla c| \) is the displacement speed, \( \vec{N} = -\nabla c/|\nabla c| \) is the local flame normal vector and \( a_T = (\delta_{ij} - N_iN_j)\partial u/\partial x_i \) is the tangential strain rate. It is possible to decompose \( S_d \) into the reaction, normal diffusion and tangential diffusion components (i.e., \( S_r, S_s, \) and \( S_t ) [8–10, 40, 41] .

\[
S_r = \frac{w}{\rho |\nabla c|}, \quad S_s = \frac{\vec{N} \cdot (\rho Dc\nabla c)}{\rho |\nabla c|}, \quad S_t = -Dc\nabla \cdot \vec{N}.
\]

(15)

It has been shown in several previous studies [5, 6, 8, 10, 25] that \( \langle \alpha_T \rangle \) remains positive throughout the flame brush and thus acts to generate flame surface area, whereas the contribution of curvature to stretch \( (\Sigma \nabla \cdot \vec{N})_s = \left[ (S_r + S_s) \nabla \cdot \vec{N}_s \right] - \left[ \frac{Dc}{Dt}(\nabla \cdot \vec{N})^2 \right] \) is primarily responsible for flame surface area destruction. The equilibrium of flame surface area generation and destruction yields \( \langle \Sigma \rangle = 0 \), which gives rise to [9]:

\[
\langle \alpha_T \rangle_s = -\left[ (S_r + S_s) \nabla \cdot \vec{N}_s \right] + \left[ \frac{Dc}{Dt}(\nabla \cdot \vec{N})^2 \right] \]

(16)

The stretch rate induced by \( -\left[ \frac{Dc}{Dt}(\nabla \cdot \vec{N})^2 \right] \) becomes the leading order sink term in the thin reaction zones regime [8–10, 42]. However, most algebraic models (e.g., FSDA, FSDC, FSDCH, and FSDW) were proposed in the CF regime based on the equilibrium of the stretch rates induced by \( \left[ (S_r + S_s) \nabla \cdot \vec{N}_s \right] \) and \( \langle \alpha_T \rangle_s \) and the flame surface area destruction due to \( -\left[ \frac{Dc}{Dt}(\nabla \cdot \vec{N})^2 \right] \) was ignored [4, 12–14]. As a result, these models underestimate the flame surface area destruction rate in the thin reaction zones regime, which leads to overprediction of \( \Sigma_{\text{gen}} \) for the FSDA, FSDC, FSDH, and FSDW models.

The disagreement between the FSDF model prediction and DNS data originates principally due to the inaccuracy in estimating \( \Gamma \) and \( D \), while the difference between the FSDK prediction and DNS data arises from inaccurate estimation of \( \eta_i \). Hence a more accurate estimation of \( \Gamma \), \( D \), and \( \eta_i \) will result in better performance of both the FSDF and FSDK models.

4.3 Performance of Models for the Variation of \( \Sigma_{\text{gen}} \). It is important to assess the models based on their ability to capture the correct variation of \( \Sigma_{\text{gen}} \) with \( \tau \) across the flame brush. The variation of mean \( \Sigma_{\text{gen}} \) conditionally averaged on \( \tau \) is shown in Figure 4 for \( \Delta = 8A_m = 0.8\delta_{\text{th}} \) and Figure 5 for \( \Delta = 24A_m = 2.4\delta_{\text{th}} \), respectively. These filter widths have been chosen since they correspond to \( \Delta < \eta_i \) and \( \Delta > \eta_i \) respectively. The following observations can be made from Figure 4 about the model predictions at \( \Delta = 8A_m = 0.8\delta_{\text{th}} \).

(i) The models FSDA, FSDC, FSDCH, FSDW, and FSDKNEW tend to capture the variation of the conditional mean value of \( \Sigma_{\text{gen}} \) with \( \tau \) obtained from DNS data. The prediction of the MFSDF model remains comparable to that of the FSDF model for \( \Delta = 8A_m = 0.8\delta_{\text{th}} \).
(ii) The FSDW model consistently overpredicts the conditional mean value of \( \Sigma_{gen} \) for all cases. The FSDW model also predicts a skewed shape, which fails to capture the trend predicted by DNS.

(iii) The model FSDK underpredicts the conditional mean value of \( \Sigma_{gen} \) in all cases. The physical explanations provided earlier for the underprediction of \( \Sigma_{gen} \) by the FSDK model is also responsible for the underprediction seen here.

A comparison between Figures 4 and 5 reveals that the predictions of the various algebraic FSD models exhibit greater spread for \( \Delta = 24 \Delta_m = 2.4 \delta_{th} \) than in the case of \( \Delta = 8 \Delta_m = 0.8 \delta_{th} \). The following observations can be made from Figure 5 about the model predictions at \( \Delta = 24 \Delta_m = 2.4 \delta_{th} \):

(i) Similar to \( \Delta = 8 \Delta_m \), the FSDW model predicts a peak at \( \tau > 0.6 \), whereas the peak value of conditionally averaged \( \Sigma_{gen} \) from DNS occurs at \( \tau = 0.5 \) for all the cases.

(ii) The models FSDW, FSDA, FSDC, and FSDCH tend to overpredict the conditionally averaged value of \( \Sigma_{gen} \) and the level of the overprediction increases with decreasing Lewis number.

(iii) The models FSDF, FSDK, FSDNEW, and MFSDF tend to predict the conditionally averaged value of \( \Sigma_{gen} \) satisfactorily throughout the flame brush.

(iv) The difference in the predictions of the models MFSDF, and FSDF seem to be very small for all the flames considered here.

The inaccuracy in the predictions of the mean value of \( \Sigma_{gen} \) conditional on \( \tau \) can be characterised once again using a percentage error (PE)

\[
\text{PE}_2 = \frac{\Sigma_{gen}^\text{MODEL} - \Sigma_{gen}^\text{DNS}}{\Sigma_{gen}^\text{MAX}} \times 100,.
\]

where \( \Sigma_{gen}^\text{MODEL} \) and \( \Sigma_{gen}^\text{DNS} \) are the mean values of \( \Sigma_{gen} \) conditional on \( \tau \) as obtained from model prediction and DNS respectively, and \( \Sigma_{gen}^\text{MAX} \) is the maximum value of conditionally averaged \( \Sigma_{gen} \) obtained from DNS. The error in the model prediction according to (16) is shown in Figure 6 for filter size \( \Delta = 8 \Delta_m = 0.8 \delta_{th} \) and in Figure 7 for filter size \( \Delta = 24 \Delta_m = 2.4 \delta_{th} \). Note that the models predicting \( \text{PE}_2 \) outside a margin of \( \pm 15\% \) have been discarded. In the case of \( \text{Le} = 0.34 \) (case A) the models FSDNEW, FSDF, MFSDF, and FSDC stay within the \( \pm 15\% \) error limit for \( \Delta = 8 \Delta_m \) whereas only the models FSDF, MFSDF, and FSDNEW remain within the \( \pm 15\% \) error limit for \( \Delta = 24 \Delta_m \). As Le increases to 0.6 (case B), the models FSDNEW, FSDC, FSDF, MFSDF, FSDC, FSDA, and FSDK predict within the \( \pm 15\% \) error margin and have been listed in terms of decreasing accuracy for \( \Delta = 8 \Delta_m \). For case B only the predictions of FSDK, FSDF, MFSDF and FSDK remain within the \( \pm 15\% \) error margin for \( \Delta = 24 \Delta_m \). In the Le = 0.8 case (case C), the models FSDF, FSDK, MFSDF, FSDC, FSDA, FSDK, and FSDK all provide predictions within \( \pm 15\% \) for \( \Delta = 8 \Delta_m \), whereas the predictions of FSDK, FSDF, MFSDF, FSDC, FSDA, and FSDK remain within \( \pm 15\% \) for \( \Delta = 24 \Delta_m \). For \( \text{Le} = 1.0 \) and 1.2 (cases D and E) the models FSDF, MFSDF, FSDK, and FSDK all present within the \( \pm 15\% \) error margin for \( \Delta = 8 \Delta_m \), whereas the models FSDF, MFSDF, FSDK, and FSDK all provide predictions within the \( \pm 15\% \) error margin for \( \Delta = 24 \Delta_m \). The model FSDK was found to predict within the \( \pm 15\% \) error margin for \( \Delta = 24 \Delta_m \) in the \( \text{Le} = 1.0 \) flame but its prediction remains marginally beyond the \( \pm 15\% \) error margin for \( \Delta = 24 \Delta_m \) for the \( \text{Le} = 1.2 \) flame considered here (The maximum magnitude of \( \text{PE}_2 \) for the FSDW model in the \( \text{Le} = 1.2 \) case is 15.2%, and the variation of \( \text{PE}_2 \) with \( \tau \) in this case is qualitatively similar to the Le = 1.0 case considered here).

Comparing the performance of the model at \( \Delta = 8 \Delta_m \) and \( \Delta = 24 \Delta_m \), it can be seen that FSDK, FSDF, and FSDK predict \( \Sigma_{gen} \) satisfactorily at \( \Delta = 8 \Delta_m \) but the agreement with DNS deteriorates at \( \Delta = 24 \Delta_m \). By contrast, the FSDK prediction is closer to DNS data at \( \Delta = 24 \Delta_m \) than at \( \Delta = 8 \Delta_m \). The models FSDF, MFSDF, and FSDKNEW fare well at both \( \Delta = 8 \Delta_m \) and \( \Delta = 24 \Delta_m \) for all the Lewis number values considered here. It is worth noting that the FSDKNEW model was designed to predict the volume-averaged value of generalised FSD (\( \Sigma_{gen} \)), but judging from Figures 4–7, this model also performs satisfactorily with respect to predicting the correct variation of \( \Sigma_{gen} \) across the flame brush.

The prediction of the model FSDK improves with increasing filter width \( \Delta \), unlike the other models, which is consistent with observations made in the context of Figure 3. The prediction of the FSDK model remains skewed towards the product side of the flame brush due to the \( \tau \) dependence of \( \Xi \) (i.e., \( \Xi = 1 + 1.24 \tilde{c}_{\text{gen}} \tilde{u}_0 / \Sigma Re_\eta \)) proposed in [12]. The FSDK, FSDW, FSDA, and FSDKCH models underestimate the destruction rate of flame surface area in the thin reaction zones regime due to the underestimation of FSD destruction arising due to the curvature stretch contribution \(-[D_s(\nabla \cdot N)^2]_f \), which eventually leads to the overprediction of conditionally averaged value of \( \Sigma_{gen} \).

4.4. Performance of Models for the Local \( \Sigma_{gen} \) Behaviour.

The FSD predicted by the models should have the correct resolved strain rate and curvature dependence in the context of LES and thus the correlation coefficient between the FSD obtained from DNS and from the model prediction should remain as close to unity as possible. The variation of the correlation coefficients between the model prediction and generalised FSD \( \Sigma_{gen} \) obtained from DNS in the range of filtered reaction progress variable 0.1 \( \leq \tau \leq 0.9 \) are shown in Figure 8 for different filter widths. The regions corresponding to 0.1 \( \leq \tau \leq 0.9 \) have been ignored since the correlation coefficients have little physical significance in these regions due to the small values of \( \Sigma_{gen} \) obtained from both DNS and model predictions. Figure 8 indicates that the correlation coefficients decrease with increasing \( \Delta \) due to increased unresolved subgrid wrinkling, which makes the local variation of \( \Sigma_{gen} \) different from \( |\nabla \tau| \). The extent of the deviation of the correlation coefficients from unity increases with decreasing Le for a given value of \( \Delta \). Figure 8
indicates that the models FSDA, FSDF, FSDK, FSDNEW, and FSDW have comparable correlation coefficients, which deviate considerably from unity for large values of $\Delta$. This indicates that algebraic models may not be able to predict FSD such that its local strain rate and curvature dependencies can be appropriately captured, especially in the TRZ regime. Hence a transport equation for FSD might need to be solved to account for the local strain rate and curvature effects on $\Sigma_{\text{gen}}$ [5, 6, 8, 10, 11].

5. Conclusions

The performance of several wrinkling factor based LES algebraic models for $\Sigma_{\text{gen}}$ has been assessed for nonunity Lewis number flames in the TRZ regime based on a DNS database of freely propagating statistically planar turbulent premixed flames with $Le$ ranging from 0.34 to 1.2. It has been found that the fractal dimension $D$ increases with decreasing $Le$, whereas $Le$ does not have any significant influence on the value of the normalised inner cut-off scale $\eta/\delta_z$. For all Lewis number cases the inner cut-off scale is found to be equal to the thermal flame thickness (i.e., $\eta/\delta_z$). Based on the analysis of DNS data, a new parameterisation of $D$ is proposed, where the effects of $Le$ are explicitly accounted for. Thus, three-dimensional DNS with detailed chemistry will be necessary, together with experimental data, for a more comprehensive assessment of LES algebraic models for $\Sigma_{\text{gen}}$.

Appendix

A. Effects of Re on Fractal Dimension $D$

The effects of $Re$ on $D$ have been analysed based on a simplified chemistry based DNS database [43, 44], in which the variation of $Re = Da^2 Ka^2$ is brought about by modifying Da and Ka independently of each other. The initial values of $u'/S_{th}$ and $l/\delta_{th}$ for all the flames in this DNS database are shown in Table 1(a) along with the values of heat release parameter $\tau = (T_{ad} - T_0)/T_0$, Damköhler number $Da = S_{th}/u' \delta_{th}$, Karlovitz number $Ka = (u'/S_{th})^{3/2}(S_{th}/\alpha T_0)^{-1/2}$, and turbulent Reynolds number $Re_t = \rho u' l/\mu_0$.

The variations of $\log[(\Sigma_{\text{gen}})/(\langle \nabla \tau \rangle)]$ with $\log(\Delta/\delta_z)$ for cases A1–E1 are shown in Figure 9, which demonstrate that $D$ is greater for flames with higher $Re_t$, and that $D$ attains an asymptotic value of 7/3 for unity Lewis number flames with high values of $Re_t$ (e.g., cases D1 and E1). The prediction of $\langle \Sigma_{\text{gen}}/(\langle \nabla \tau \rangle) \rangle = (\Delta/\eta_0)^{D-2}$ with $\eta_0$ obtained from DNS and $D$ obtained from (11) is also shown in Figure 9, which indicates that (11) satisfactorily captures the slope of the best-fit straight line.

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References


