Modelling of the strain rate contribution to the FSD transport for non-unity Lewis number flames in LES

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1 Introduction

Flame Surface Density (FSD) based modelling is one of the well-established reaction rate closures for turbulent premixed combustion in the context of Reynolds Averaged Navier Stokes (RANS) simulations [1,2] and this approach is becoming increasingly popular in the context of Large Eddy Simulations (LES) [3,4]. The generalised FSD Σ_{gen} is defined as: $\Sigma_{gen} = \overline{|\nabla c|}$ [3], where c is the reaction progress variable, and the overbar indicates a Reynolds averaging/LES filtering operation as appropriate. The exact transport equation of Σ_{gen} is given by [4-6]:

$$\partial\Sigma_{gen}/\partial t + \partial(\tilde{u}_j\Sigma_{gen})/\partial x_j = -\partial[(\overline{(u_j)}_s - \tilde{u}_j)\Sigma_{gen}]/\partial x_j + \overline{[(\delta_{ij} - N_iN_j)\partial u_i/\partial x_j]}_s\Sigma_{gen} + \overline{(S_d\nabla.\vec{N})}_s\Sigma_{gen} - \nabla.(\overline{(S_d\vec{N})}_s\Sigma_{gen}) \quad (1)$$

where u_j is the j^{th} component of velocity, $N_i = -(\partial c/\partial x_i)/|\nabla c|$ is the i^{th} component of flame normal vector, $S_d = (Dc/Dt)/|\nabla c|$ is the displacement speed and $\overline{(Q)}_s = \overline{Q|\nabla c|}/\Sigma_{gen}$ is the surface-weighted filtered value of a general quantity Q in the context of LES. The first term on the left had side of Eq. 1 is the transient term whereas the second term represents the mean advection of Σ_{gen}. The terms on right hand side of Eq. 1 represent the contributions of sub-grid turbulent transport, tangential strain rate, flame curvature and flame propagation to the FSD transport and these terms are commonly referred to as the FSD transport, strain rate, curvature and propagation terms respectively. All the terms on the right hand side of Eq. 1 are unclosed, and thus need modelling. The present work will only focus on the modelling of the strain rate term $\overline{(a_T)}_s\Sigma_{gen} = \overline{[(\delta_{ij} - N_iN_j)\partial u_i/\partial x_j]}_s\Sigma_{gen}$, where $a_T = (\delta_{ij} - N_iN_j)\partial u_i/\partial x_j$ is the tangential strain rate. Interested readers are referred to Ref. [5] for the discussion on the modelling of the sub-grid transport, curvature and propagation terms. To date, most FSD based closures [1-6] have been proposed for flames without differential diffusion effects of heat and mass. The differential diffusion of heat and mass in flames can be characterized in terms of Lewis number Le, which is defined as the ratio of thermal diffusivity α_T to mass diffusivity D (i.e. $Le = \alpha_T/D$). The effects of differential diffusion arising due to non-unity Lewis number on the FSD transport have rarely been analysed in existing literature [7]. Recently non-unity Lewis number effects on Σ_{gen} were analysed by Chakraborty and Cant [7] in the context of RANS based on an *a-priori* analysis of Direct Numerical Simulations (DNS) data. However, the effects of Le on the statistical behaviours of $\overline{(a_T)}_s\Sigma_{gen}$ are yet to be addressed in detail, and this paper addresses this gap in the existing literature. In this respect, the main objectives of this analysis are: (i) to demonstrate the effects of Le on the statistical behaviours of $\overline{(a_T)}_s\Sigma_{gen}$ using a DNS database of freely propagating statistically planar flames with Le ranging from 0.34 to 1.2 and (ii) to assess the performances of the existing models for $\overline{(a_T)}_s\Sigma_{gen}$ in the context of LES with respect to the FSD strain rate term extracted from explicitly filtered DNS data.

2 Mathematical Background and Numerical Implementation

For the purpose of modelling $\overline{(a_T)}_s\Sigma_{gen}$ is often split in the following manner [4,5]: $\overline{(a_T)}_s\Sigma_{gen} = S_m + S_{hr} + S_{sg}$ where S_m, S_{hr} and S_{sg} are the contributions arising from the resolved velocity gradient, heat release and sub-grid processes, which are defined as [4,5]:

$$S_m = (\delta_{ij} - \overline{(N_i N_j)}_s)\frac{\partial \tilde{u}_i}{\partial x_j}\Sigma_{gen};\; S_{hr} = -\tau(K - \tilde{c})\frac{\overline{(\rho S_d)}_s}{\rho_0}\frac{\partial \overline{(N_i)}_s}{\partial x_i}\Sigma_{gen};\; S_{sg} = \overline{(a_T)}_s\Sigma_{gen} - (S_m)_M - S_{hr} \quad (2i)$$

$$(S_m)_M = [(\delta_{ij} - n_{ij})\partial\tilde{u}_i / \partial x_j]\Sigma_{gen} \quad (2ii)$$

where $\tau = (T_{ad} - T_0)/T_0$ is the heat release parameter with T_{ad} and T_0 being the adiabatic flame, and unburned gas temperatures respectively and K is a parameter which depends on the choice of c isosurface which represents the flame surface [4]. Here the local value of c is considered to represent K following a previous analysis [5]. It can be seen from Eq. 2 that $\overline{(N_i N_j)}_s$ needs to be modelled in order to evaluate S_m and $\overline{(N_i N_j)}_s$ is evaluated here by extending the RANS model proposed by Cant *et al.* [1] in the following manner: $\overline{(N_i N_j)}_s = \overline{(N_i)}_s\overline{(N_j)}_s + (\delta_{ij}/3)[1 - \overline{(N_k)}_s\overline{(N_k)}_s]$. In Eq. 2 $(S_m)_M$ refers to the modelled expression of S_m where n_{ij} refers to the modelled expression of $\overline{(N_i N_j)}_s$. Equation 2 further suggests that the magnitude of S_{sg} depends on the expressions used for S_m and S_{hr}. The sub-grid strain rate term S_{sg} is modelled in the following manner in Refs. [4,5]:

$$S_{sg} = \Phi\,\Gamma(u'_\Delta/\Delta)\Sigma_{gen} \quad (3)$$

where $u'_\Delta = \sqrt{[\overline{(\rho u_i u_i)}/\bar{\rho} - \tilde{u}_i\tilde{u}_i]/3}$ is the sub-grid turbulent velocity fluctuation, Δ is the LES filter width, Φ is a model parameter, Γ is an efficiency function which is a function of $\sqrt{\tilde{k}}/S_L$ and $\Delta S_L/\alpha_{T0}$ [8,9] with S_L and α_{T0} being the unstrained laminar burning velocity and thermal diffusivity in unburned gases respectively. The efficiency functions Γ proposed by Charlette *et al.* [8] and Angelberger *et al.* [9] have been used by Hawkes and Cant [4] for the modelling of S_{sg}. The performances of the above models for S_m and S_{sg} for non-unity Lewis number flames have been assessed here using a compressible three-dimensional DNS database of freely propagating turbulent premixed flames with global Lewis numbers Le = 0.34 , 0.6, 0.8, 1.0 and 1.2. In all cases a single-step Arrhenius type chemical reaction is taken to represent the combustion process. The simulation domain has been taken to be $24.1\delta_{th} \times 24.1\delta_{th} \times 24.1\delta_{th}$ (where $\delta_{th} = (T_{ad} - T_0)/Max|\nabla T|_L$ is the thermal flame thickness with T being the instantaneous dimensional temperature and subscript 'L' refers to quantities in unstrained planar laminar flame), which is discretised using a uniform grid of

$230 \times 230 \times 230$ ensuring about 10 grid points within δ_{th} in all cases. The heat release parameter τ, initial values of normalised root-mean-square turbulent velocity fluctuation u'/S_L and the integral length scale to flame thickness ratio l/δ_{th} are taken to be 4.5, 7.5 and 2.45 respectively for all cases considered here. Standard values of Prandtl number (i.e. Pr = 0.7), ratio of specific heats (i.e. $C_p/C_v = 1.4$) and Zel'dovich number (i.e. $\beta = 6.0$) are considered. The statistics were extracted after $3.34l/u'$ which corresponds to δ_{th}/S_L. The DNS data is explicitly filtered using a Gaussian filter using the following convolution operation: $\overline{Q(\vec{x})} = \int Q(\vec{x}-\vec{r})G(\vec{r})d\vec{r}$ where Q is a general variable. A range of filter sizes ranging from $\Delta = 0.4\delta_{th}$ to $\Delta = 2.4\delta_{th}$ has been explored, as $\Delta = 0.4\delta_{th}$ provides a limiting condition of flame being almost resolved and $\Delta = 2.41\delta_{th}$ is comparable to the integral length scale l where LES tends towards RANS simulations.

3 Results and Discussion

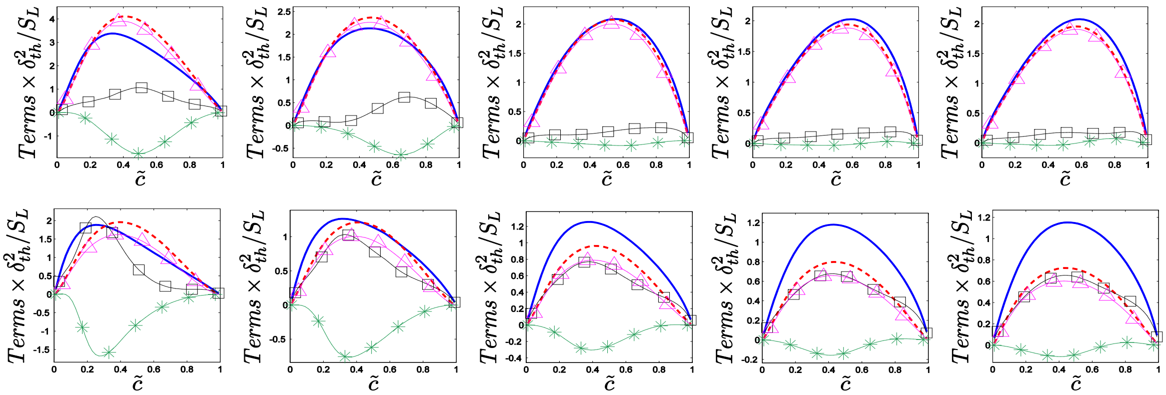

Figure 1: Variation of mean values of $\overline{(a_T)}_s\Sigma_{gen}$ (blue solid line), S_m (red dashed line), $(S_m)_M$ (magenta line with triangles), S_{hr} (green line with asterisks) and S_{sg} (black line with squares) conditional on $\tilde{c}$ across the flame brush at $\Delta \approx 0.8\delta_{th}$ (1st row) and $\Delta \approx 2.4\delta_{th}$ (2nd row) for $Le = 0.34$ (1st column), 0.6 (2nd column), 0.8 (3rd column), 1.0 (4th column) and 1.2 (5th column) cases. All the strain rate terms in this and subsequent figures are normalised by S_L/δ_{th}^2 of the respective cases.

The variations of the mean values of $\overline{(a_T)}_s\Sigma_{gen}$, S_m, S_{hr} and S_{sg} conditional on $\tilde{c}$ values for $\Delta = 0.8\delta_{th}$ and $\Delta = 2.41\delta_{th}$ for $Le = 0.34$, 0.6, 0.8, 1.0 and 1.2 flames are shown in Fig. 1. It is evident from Fig. 1 that the contributions of $\overline{(a_T)}_s\Sigma_{gen}$ and S_m remain positive throughout the flame brush for all cases considered here. The maximum magnitude of $\overline{(a_T)}_s\Sigma_{gen}$ decreases with increasing Δ as the weighted averaging process associated with LES filtering acts to decrease the peak magnitude of $\overline{(a_T)}_s\Sigma_{gen}$ with increasing Δ. It can further be seen from Fig. 1 that the relative contribution of S_m (S_{sg}) to $\overline{(a_T)}_s\Sigma_{gen}$ decreases (increases) with increasing Δ as the physical process occur increasingly at the sub-grid scale with an increase in filter width. It can be seen from Fig. 1 that the contribution of S_{hr} remains negative in the middle of the flame brush for $\Delta >> \delta_{th}$, although small positive values can be discerned on both unburned and burned gas sides. It is evident from Fig. 1 that the magnitude of S_{hr} increases with decreasing Le due to high magnitudes of $\overline{(\rho S_d)}_s$ for small values of Le as demonstrated in Ref. [7] in the context of RANS. The contribution of S_{sg} remains positive throughout the flame brush for the $Le = 0.6$, 0.8, 1.0 and 1.2 cases but the variation of S_{sg} towards the burned gas side of the flame brush for the $Le = 0.34$ case remains qualitatively different in comparison to the other cases considered here. Moreover, the peak magnitudes of S_{sg} in the $Le = 0.8, 1.0$ and 1.2 cases are obtained near the middle of the flame brush. For these cases the peak magnitude location remains skewed slightly towards the burned gas side of the flame brush for small values of Δ (i.e. $\Delta < \delta_{th}$) but the peak value location shifts towards the middle of the flame brush (i.e. $\tilde{c} \approx 0.5$) with increasing filter size Δ. By contrast, the peak magnitude of S_{sg} for the $Le = 0.34$ case takes place towards the middle of the flame brush for small filter widths (i.e. $\Delta < \delta_{th}$) but for $\Delta > \delta_{th}$ the peak value location shifts towards the unburned gas side of the flame brush (i.e. $\tilde{c} < 0.5$). The tangential strain rate term $\overline{a_T|\nabla c|}$ can be expressed as: $\overline{(a_T)}_s \Sigma_{gen} = \overline{(e_\alpha \sin^2 \alpha + e_\beta \sin^2 \beta + e_\gamma \sin^2 \gamma)|\nabla c|}$ where e_α, e_β and e_γ are the most extensive, intermediate and the most compressive principal strain rates and their angles with ∇c are given by α, β and γ respectively. It has been demonstrated by Chakraborty *et al.* [10] the extent of ∇c alignment with e_α (e_γ) increases (decreases) with decreasing Le due to strengthening of the strain rate induced by augmented heat release (arising from thermo-diffusive instability for $Le << 1$ flames) in comparison to the turbulent straining. This tendency is prevalent in the reaction zone (which occurs close to the burned gas side of the flame brush) due to strong heat release rate leading to high probability of finding $\sin^2 \alpha \approx 0$. Thus the preferential alignment of ∇c with e_α, acts to reduce the positive magnitude of S_{sg} towards the burned gas side for the $Le = 0.34$ case.

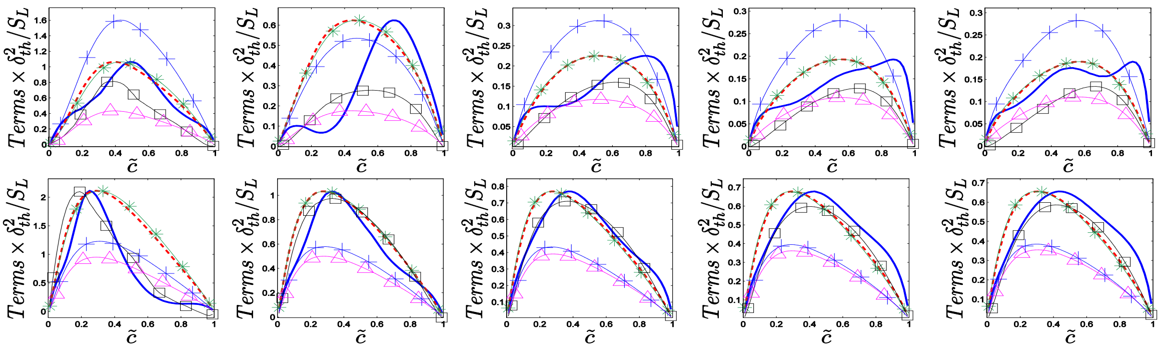

Figure 2. Variation of the mean values S_{sg} (———) conditional on $\tilde{c}$ across the flame brush along with the predictions of Eq. 3 with Γ according to Charlette *et al.* [8] with $\Phi = 1.0$ (—△—) and optimum value of Φ (see Fig. 3) (– – –), Eq. 3 with Γ according to Angelberger *et al.* [9] with $\Phi = 1.0$ (—+—) and optimum value of Φ (see Fig. 3) (—✳—) and Eq. 4 (—□—) at $\Delta \approx 0.8\delta_{th}$ (1st row) and $\Delta \approx 2.4\delta_{th}$ (2nd row) for $Le = 0.34$ (1st column), 0.6 (2nd column), 0.8 (3rd column), 1.0 (4th column) and 1.2 (5th column) cases.

The variations of the mean values of S_m and $(S_m)_M$ conditional on $\tilde{c}$ values for $\Delta = 0.8\delta_{th}$ and $\Delta = 2.4\delta_{th}$ for $Le = 0.34$, 0.8, 1.0 and 1.2 flames are also shown in Fig. 1 where $\overline{(N_i N_j)}_s$ is modelled as: $n_{ij} = \overline{(N_i)}_s \overline{(N_j)}_s + (\delta_{ij}/3)[1 - \overline{(N_k)}_s \overline{(N_k)}_s]$ [1,4]. It is evident from Fig. 1 that $(S_m)_M$ underpredicts S_m for all filter widths for all cases and the level of this underprediction increases with increasing Δ. It is worth noting that the inaccuracies involved in the modelling of $\overline{(N_i N_j)}_s$ also contributes to the magnitude of S_{sg}. The variations of the mean values of S_{sg} conditional on $\tilde{c}$ values for $\Delta = 0.8\delta_{th}$

and $\Delta = 2.4\delta_{th}$ for $Le = 0.34$, 0.6, 0.8, 1.0 and 1.2 flames are shown in Fig. 2 along with the prediction of the model given by Eq. 3. Hawkes and Cant [4] proposed $\Phi = 1.0$ for their model but Fig. 3 suggests that Eq. 3 with $\Phi = 1.0$ significantly underpredicts the magnitude of S_{sg} for all filter widths for both Charlette *et al.* [8] and Angelberger *et al.* [9] efficiency functions. However, an optimum choice of the model parameter Φ gives rise to satisfactory quantitative and qualitative predictions of S_{sg} in the $Le = 0.6$, 0.8, 1.0 and 1.2 cases considered here. However, Eq. 3, for the optimum value of Φ which matches the peak magnitude of S_{sg} obtained from DNS, fails to capture the qualitative behaviour of S_{sg} in the $Le = 0.34$ case and significantly overpredicts the magnitude of S_{sg} towards the burned gas side of the flame brush. Moreover, the optimum value of Φ for both Charlette *et al.* [8] and Angelberger *et al.* [9] efficiency functions are strongly influenced by Le, which can be substantiated from Fig. 3. The optimum values of Φ have been found to increase with decreasing Le. The optimum value of Φ for Γ proposed by Charlette *et al.* [8] does not exhibit any monotonic trend, whereas Φ for Γ proposed by Angelberger *et al.* [9] increases with increasing Δ. Here a new model for S_{sg} has been proposed as:

$$S_{sg} = \beta_1 \tilde{c}^a \Gamma(u'_\Delta/\Delta)\Sigma_{gen} - \beta_2(\tau S_L/\delta_{th})[1.0 - \overline{(N_k)}_s \overline{(N_k)}_s]\Sigma_{gen}/(1+Ka_\Delta)^b \quad (4)$$

where β_1 and β_2 are the model parameters, Γ is taken to be $\Gamma = 0.75\exp[-1.2(u'_\Delta/S_L)^{-0.3}](\Delta S_L/\alpha_{T0})^{2/3}$ according to Angelberger *et al.* [9] and $Ka_\Delta = 6.66(u'_\Delta/S_L)^{3/2}(\Delta/\delta_{th})^{-1/2}$ can be taken to be the sub-grid scale Karlovitz number. In Eq. 4 the first term on the right hand side is similar to Eq. 3 and $\tilde{c}^a$ is introduced to capture the correct qualitative behaviour across the flame brush. The second term on the right hand side of Eq. 4 arises due to the local alignment of ∇c with the most extensive principal strain rate e_α under the action of heat release, which tends to destroy flame surface area [10,11]. The prediction of Eq. 4 for $b = 0.35$ and optimum values of a, β_1 and β_2 are shown in Fig. 2. The optimum values of a, β_1 and β_2 are shown in Fig. 3, which shows that these model parameters also remain functions of Δ and Le. The model parameters a, β_1 and β_2 can be satisfactorily parameterised as (see Fig. 3):

$$a = 0.3/\{1+[\exp(-5.9(Le-0.58))]^{5.9}\} \quad (5i)$$

$$\beta_1 = k/[1+[\exp(-(\Delta/\delta_{th}-1.37))]^2] \text{ where } k = 3.2+6.21\exp(-4.74Le^{2.31}) \quad (5ii)$$

$$\beta_2 = [0.3+7.2\exp(-13.7Le^{3.47})]\times\left\{2.0-\frac{1.0}{1+[\exp(-15.0(P_2-3.3))]^2}\right\} \text{ where } P_2 = \frac{\mathrm{Re}_{t\Delta}^{0.83}+0.1}{(\Delta/\delta_{th})^{1.73}+0.1} \quad (5iii)$$

where $\mathrm{Re}_{t\Delta} = 4.0(\rho_0 u'_\Delta \Delta/\mu_0)$ can be taken as the sub-grid turbulent Reynolds number. According to Eq. 5iii β_2 increases with decreasing *Le* which accounts for strengthening of flame surface destruction due to increased extent of alignment of $|\nabla c|$ with e_α in small Lewis number flames (e.g. $Le \ll 1$) under the action of strong strain rate induced by augmented heat release arising from thermo-diffusive instabilities. It is evident from Fig. 2 that the model given by Eq. 4 satisfactorily captures both qualitative and quantitative behaviours of S_{sg} for all cases including the $Le = 0.34$ case for all values of Δ considered here.

4 Conclusions

A single step chemistry based three-dimensional DNS database of statistically planar turbulent premixed flames with global Lewis number *Le* ranging from 0.34 to 1.2 has been used to analyse the statistical behaviours of the strain rate contribution to the FSD transport in the context of LES. It has been found that *Le* has a significant influence on the statistical behaviours of S_{sg}, especially for *Le*<<1 flames. The existing models do not capture the qualitative behaviours of the sub-grid strain rate term S_{sg} for *Le*<<1 flames. Here a new model has been proposed based on *a-priori* analysis of explicitly filtered DNS data, which has been demonstrated to capture both the qualitative and quantitative behaviours of S_{sg} for all values of Δ for flames with *Le* ranging from 0.34 to 1.2. The proposed model needs to be implemented in actual LES simulations for a configuration in which experimental data is available for the purpose of *a-posteriori* assessment.

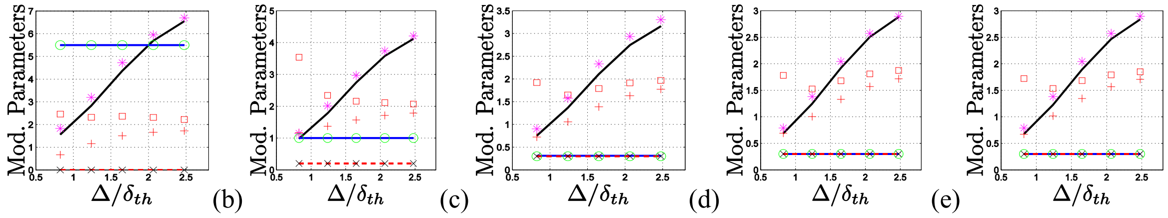

Figure 3. Variations of optimum values of *a* (×), Eq. 5i (▬ ▬ ▬), β_1 (✳), Eq. 5ii(———), β_2 (○), Eq. 5iii (———), Φ for the efficiency function by Charlette *et al.* [8] (□) and Φ for the efficiency function by Angelberger *et al.* [9] (+) with Δ/δ_{th} for: (a) $Le = 0.34$, (b) 0.6, (c) 0.8, (d) 1.0 and (e) 1.2 cases.

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