

Modelling of non-unity Lewis number effects on scalar dissipation rate transport in turbulent premixed flames

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Abstract

The influences of Lewis number Le on the transport of the scalar dissipation rate of reaction progress variable is studied using DNS data of freely propagating turbulent premixed flames with Le ranging from 0.34 to 1.2. A transport equation for the Favre averaged dissipation rate is derived for non-unity Le flames and the statistical behaviours of the unclosed terms in that transport equation are studied in detail using DNS data and their closure models are proposed. The effects of dilatation rate become increasingly strong with decreasing Le because of thermo-diffusive instabilities. The resulting strong acceleration in the flame normal direction leads to counter-gradient transport for turbulent flux of the dissipation rate when $Le < 1$. The alignment behaviour of the scalar gradient vector with the local principal strain rates is found to be strongly affected by the global Lewis number Le . The new models proposed in this study duly account for these effects of Le on scalar dissipation rate transport.

Introduction

Scalar dissipation rate has a central importance in turbulent reacting flows [1]. Its modelling has mostly been studied for non-premixed flames although the mean reaction rate is proportional to Favre averaged scalar dissipation rate in turbulent premixed flames [2]. However, there have been few studies on this topic for unity Lewis number flames [3-8]. The instantaneous scalar dissipation rate is defined as $N_c \equiv D(\nabla c \bullet \nabla c)$, where c is the reaction progress variable and D is its diffusivity. The Lewis number is defined as the ratio of thermal diffusivity α_T to D . In the context of turbulent premixed flames one requires to model the Favre averaged scalar dissipation rate in order to model the mean reaction rate. However, the contribution from the gradient of Favre averaged progress variable \tilde{c} is often negligible in the RANS context and one needs to model $\overline{\rho \tilde{\epsilon}_c} = \overline{\rho D \nabla c'' \cdot \nabla c''}$, where the double prime denotes the Favre fluctuation of c and the over-bar and tilde indicate Reynolds and Favre averaging operations respectively. Moreover, the scalar dissipation rate is closely related to the generalised Flame Surface Density (FSD) $\Sigma_{gen} = |\overline{\nabla c}| = \overline{(N_c / D)^{1/2}}$, which is often used for reaction rate closure in turbulent premixed flames [5, 9].

To date, all existing models of the mean dissipation rate $\tilde{\epsilon}_c$ in turbulent premixed flames do not include differential diffusion effects, which is characterised by non-unity Le . A recent study [10] showed that the differential diffusion of heat and mass can significantly influence the physical processes determining the evolution of ∇c , and therefore N_c . The predominant effect comes due to heat release and its associated influences on the turbulence-scalar-chemistry interactions. A close understanding of these influences is yet to be obtained so that accurate models for the scalar dissipation rate transport can be developed.

However, it is to be noted that the influences of Le on scalar gradient transport in turbulent premixed flames have rarely been investigated [10, 11] Thus, the main objectives here are as follows:

1. To understand the influences of Le on various unclosed terms in the $\tilde{\epsilon}_c$ transport equation.
2. To construct Reynolds Averaged Navier Stokes (RANS) models for these terms, including the non-unity Lewis number effects.

The above objectives are addressed using compressible three-dimensional Direct Numerical Simulation (DNS) data of a number of freely propagating statistically planar turbulent premixed flames having the same initial turbulent flow field parameters and Le ranging from 0.34 to 1.2.

The rest of the paper is organised as follows. The mathematical background is presented in the next section followed by a brief discussion on numerical implementation. Following this, results are presented and discussed. Finally main findings are summarised and conclusions are drawn.

Mathematical Background

Although it is desirable to have both three dimensionality of the turbulence and detailed chemistry for combustion kinetics, the computational requirements for DNS limits the simulations, until recently, either to two dimensions with detailed chemistry or to three-dimensions with simplified chemistry. As three dimensionality of the gradient information is to be retained for our analysis, a single irreversible reaction with Arrhenius rate expression is used for combustion chemistry. The reaction progress variable c is defined using reactant mass fraction Y_R in the following manner so that c increases monotonically from zero in fresh gases to unity in fully burned products:

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$$c \equiv (Y_{R0} - Y_R)/(Y_{R0} - Y_{R\infty}) \quad (1)$$

The subscripts 0 and ∞ are used to denote values in fresh reactants and fully burned products respectively. For unity Le flames at low Mach number c in Eq.(1) is equivalent to the one based on normalised temperature $T=(\tilde{T}-T_0)/(T_{ad}-T_0)$ where \tilde{T} is the dimensional temperature, T_0 is the fresh gas temperature and T_{ad} is the adiabatic flame temperature. However, in non-unity Le flames, the temperature can be super-adiabatic (i.e. $T>1$) [12, 13] whereas Eq. (1) ensures that $0 \leq c \leq 1$. Using the transport equation for c , it is possible to obtain a transport equation for $\tilde{\varepsilon}_c$ neglecting the terms originating from the gradients of D [5]:

$$\bar{\rho} \frac{\partial \tilde{\varepsilon}_c}{\partial t} + \bar{\rho} \tilde{u}_j \frac{\partial \tilde{\varepsilon}_c}{\partial x_j} = \frac{\partial}{\partial x_j} \left[\rho D \frac{\partial \varepsilon_c}{\partial x_j} \right] + \underbrace{T_{11} + T_{12}}_{T_1} + \underbrace{T_2 + T_{31} + T_{32} + T_{33}}_{T_3} + T_4 - D_2 \quad (2)$$

The physical meanings of the various terms in Eq. (2) are as follows. The first term is the transient term and the second term is the mean advection term. The first term on the RHS is the molecular diffusion of the mean dissipation rate. The term T_1 indicates turbulent transport of the scalar dissipation rate and T_2 arises due to heat release. The term T_3 is the turbulence-scalar interaction term containing the physical information on the alignment of ∇c with the local principal strain rates [6-8,10]. The contributions of chemical reaction and the molecular dissipation of $\tilde{\varepsilon}_c$ are denoted by T_4 and $-D_2$ respectively. The terms T_1 to T_4 are unclosed and are to be modeled. A scaling analysis [5] suggested that T_2 , T_{32} , T_4 and D_2 are at the leading order for all values of the Damköhler number, $Da \equiv l S_L / u' \delta_{th}$ and the turbulent Reynolds number, $Re_t \equiv \rho_0 u' l / \mu$, where l is the integral length scale, u' is the initial rms value of turbulent velocity fluctuation, ρ_0 is the fresh gas density and $\delta_{th} = (T_{ad} - T_0) / \max |\nabla \tilde{T}|_L$ is the thermal thickness of the laminar flame in which subscript L denotes steady unstrained laminar flame value.

Numerical Implementation

The simulations have been carried out using a well proven code, SENGA, in a cubic domain with length of each side equal to $24 \delta_{th}$. The domain is discretised using $230 \times 230 \times 230$ grid points uniformly in all three directions. The computational boundaries are taken to be partially non-reflecting in the direction of mean flame propagation and periodic in transverse directions. The spatial derivatives are evaluated using a 10th order central difference scheme with order of differentiation gradually reducing to one-sided 2nd order scheme near non-periodic boundaries. The time advancement is carried out using a low storage 3rd order Runge-Kutta scheme. The turbulence field is initialised using standard pseudo-spectral method. The flame is initialised using an unstrained steady planar laminar flame with about 10 grid points inside $\min(\delta_{th}, \delta_L)$. The slope thickness $\delta_L \equiv 1 / \max |\nabla c|_L$ is larger (smaller) than

the thermal thickness δ_{th} for flames with $Le < 1$ ($Le > 1$) and they are equal when $Le = 1$. The pre-exponential factors for the single-step reaction are chosen so that the unstrained laminar flame speed S_L and its thermal thickness δ_{th} remain the same for all Le flames while the values of the specific heat, the thermal conductivity, the density-weighted mass diffusivity and the Zel'dovich number $\beta \equiv T_{ac}(T_{ad} - T_0)/T_{ad}^2 = 6$ are kept unaltered. The heat release parameter is $\tau \equiv (T_{ad} - T_0)/T_0 = 4.5$. The standard values are taken for Prandtl number ($Pr = 0.7$) and ratio of specific heats ($\gamma = 1.4$). For the sake of simplicity the thermo-physical properties are taken to be independent of temperature while the Le is set to 0.34, 0.8, 1.0 and 1.2 respectively for four different turbulent flames. Table 1 lists the various attributes of the DNS flames. The initial values of normalised turbulent velocity fluctuation, normalised integral length scale, the Damköhler number Da , the Karlovitz number $Ka = (u'/S_L)^{3/2} (l/\delta_{th})^{-1/2}$ and the turbulent Reynolds number Re_t are the same. However, the thickness ratio δ_L/δ_{th} are different for different Lewis number flames. It is to be noted that the Ka is greater than unity, which implies that the combustion in all the flames belong to the thin reaction zones regime [17]. In general, these simulations should be run for a time $t_{sim} = \max(t_f, t_c)$ when the turbulence is decaying, where $t_f \equiv l/u'$ is the initial eddy turn over time and $t_c \equiv \delta_{th}/S_L$ is the chemical time scale. All the simulations have been run for about three initial eddy turn over times which correspond to about one chemical time scale. It is admitted that the simulation time remains small but several previous studies [5-8, 10-13] with similar or smaller simulation time contributed significantly to turbulent combustion modelling in the past.

Le	u'/S_L	δ_L/δ_{th}	l/δ_{th}	Re_t	Da	Ka
0.34	7.5	2.17	2.45	47	0.33	13
0.8	7.5	1.15	2.45	47	0.33	13
1.0	7.5	1.0	2.45	47	0.33	13
1.2	7.5	0.90	2.45	47	0.33	13

Table 1: Attributes of DNS database

Data processing

All the terms in the RHS of Eq.(2) are obtained from DNS data by ensemble averaging relevant quantities over a number of transverse planes in the direction of mean flame propagation. For the statistically planar flames Eq.(2) becomes

$$\bar{\rho} \frac{\partial \tilde{\varepsilon}_c}{\partial t} + \bar{\rho} \tilde{u}_1 \frac{\partial \tilde{\varepsilon}_c}{\partial x_1} = \frac{\partial}{\partial x_1} \left[\rho D \frac{\partial \varepsilon_c}{\partial x_1} \right] + T_1 + T_2 + T_3 + T_4 - D_2 \quad (3a)$$

where

$$T_1 = - \frac{\partial(\bar{\rho} u'_1 \varepsilon_c)}{\partial x_1} - 2 \rho D u'_1 \left(\frac{\partial c''}{\partial x_1} \right) \left(\frac{\partial^2 \tilde{c}}{\partial x_1 \partial x_1} \right) \quad (3b)$$

$$T_2 = -2D \frac{[\dot{w} + \nabla \cdot (\rho D \nabla c)]}{\rho} \frac{\partial c}{\partial x_k} \frac{\partial \rho}{\partial x_k} + 2 \frac{\bar{D}}{\bar{\rho}} \frac{\partial \tilde{c}}{\partial x_1} \frac{\partial \bar{\rho}}{\partial x_1} \left[\dot{w} + \nabla \cdot (\rho D \nabla c) - \frac{\partial(\bar{\rho} u'_1 c'')}{\partial x_1} \right] \quad (3c)$$

$$T_3 = -2\rho D \frac{\partial \tilde{c}}{\partial x_i} \frac{\partial \overline{u_i'' c''}}{\partial x_k} \frac{\partial c''}{\partial x_k} - 2\rho D \frac{\partial c''}{\partial x_j} \frac{\partial \overline{u_j'' c''}}{\partial x_k} \frac{\partial c''}{\partial x_k} \quad (3d)$$

$$-2\rho D \frac{\partial c''}{\partial x_i} \frac{\partial c''}{\partial x_i} \frac{\partial \tilde{u}_i}{\partial x_1} = T_{31} + T_{32} + T_{33} \quad (3e)$$

$$T_4 = 2D \frac{\partial \tilde{w}}{\partial x_k} \frac{\partial c}{\partial x_k} - 2D \frac{\partial \tilde{w}}{\partial x_1} \frac{\partial \tilde{c}}{\partial x_1} \quad (3f)$$

$$D_2 = 2\rho D^2 \frac{\partial^2 c''}{\partial x_k \partial x_i} \frac{\partial^2 c''}{\partial x_k \partial x_i} \quad (3f)$$

The statistical convergences of the results are assessed by halving the samples in the transverse direction. The qualitative and quantitative agreement of the results obtained using the half and full sample sizes are found to be satisfactory. Thus, the results are deemed to be statistically converged and those discussed in the next sections are obtained using full samples.

Results and Discussion

The variations of the normalised mean dissipation rate with \tilde{c} for three different Le flames are shown in Fig.1. The variation of the mean dissipation rate observed is consistent with previous DNS [5, 8] and experimental results [18]. The maximum value of $\tilde{\varepsilon}_c$ decreases with increasing Le .

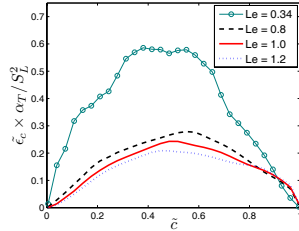


Fig. 1: Variations of $\tilde{\varepsilon}_c$ across the flame brush.

As shown in Eq.(3), the evolution of $\tilde{\varepsilon}_c$ is governed by the various sources and sinks and thus its Le dependence will also be dictated by the influences of Le on these source and sink terms. Their variations across the flame brush are shown in Fig.2. The contribution from chemical reaction rate, T_4 remains a dominant source whereas the dissipation term ($-D_2$) acts as the dominant sink for all the flames studied here. However, the decrease in their magnitudes with increasing Le is to be noted. The second dominant source is T_2 and its relative magnitude increases with decreasing Le . For the small Le flame, the magnitude of turbulence-scalar interaction term, T_3 , is significantly greater than that in the unity Le flame. Furthermore, this term makes a negative contribution for the $Le < 1$ flames, whereas it is positive towards the leading side and negative towards the trailing side for the $Le \geq 1$ flames, which is consistent with earlier findings [10]. Although T_3 contribution seems small in Fig.2, T_{32} is a physically important term and a careful analysis shows that its contribution can be as large as T_2 contribution in some flames [5]. The above findings are consistent with scaling arguments [5] and previous DNS results [7,8]. It is also to be noted

that the contribution of T_1 remains negligible compared to other terms. The effects of Le on the modelling of T_1 , T_2 , T_3 , T_4 and ($-D_2$) will be studied next.

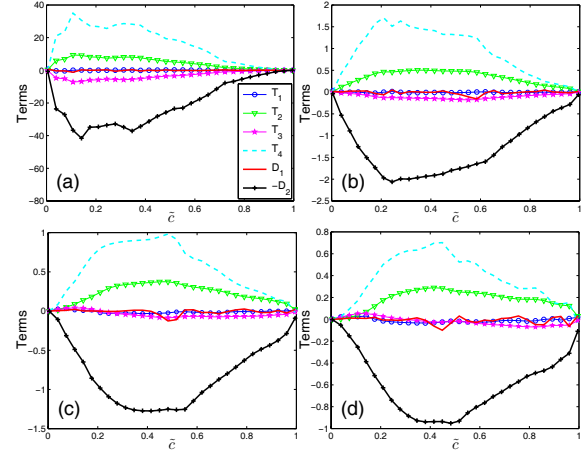


Fig. 2: Behaviour of various source and sink terms in Eq.(3) for (a) $Le = 0.34$, (b) $Le= 0.8$, (c) $Le= 1.0$ and (d) $Le=1.2$ flames. The terms in this and subsequent figures are normalised with respect to $\rho_0 S_L^4 / \alpha_T^2$ of respective flames.

Modelling of turbulent transport of $\tilde{\varepsilon}_c$

According to Ref. [5], the order of magnitude for the ratio of T_{11} to T_{12} is of the order of Re_t thus T_{12} contribution is negligible compared to T_{11} in high Re_t flows. This is found to apply for the DNS flames, although their Re_t are not very high. As a result of this, T_1 becomes

$$T_1 \approx T_{11} = -\partial(\rho u_j'' \varepsilon_c) / \partial x_j \quad (4a)$$

Often the turbulent flux of the dissipation rate is modelled assuming gradient transport as follows:

$$\rho u_j'' \varepsilon_c = -(\mu_t / \sigma_\varepsilon) \partial \tilde{\varepsilon}_c / \partial x_j \quad (4b)$$

where μ_t is the eddy viscosity and σ_ε is an appropriate turbulent Schmidt number. According to this model, a negative (positive) value of $\overline{\rho u_i'' \varepsilon_c} \times \partial \tilde{\varepsilon}_c / \partial x_i$ indicates the gradient (counter gradient) transport. The present DNS database reveals that $\overline{\rho u_i'' c''}$ exhibits counter gradient transport in the $Le = 0.34$ flame and gradient transport is observed in the flames with $Le \geq 1$. Both gradient and counter-gradient transport are observed for the $Le=0.8$ flame. This counter gradient transport of $\overline{\rho u_i'' c''}$ is a consequence of higher rate of burning and strong flame normal acceleration in the flames with $Le \ll 1$ due to thermo-diffusive instability. It has been found that $\overline{\rho u_i'' \varepsilon_c}$ shows counter-gradient transport when $\overline{\rho u_i'' c''}$ is counter-gradient in nature. A model for $\overline{\rho u_i'' \varepsilon_c}$ is proposed as:

$$\overline{\rho u_i'' \varepsilon_c} = \lambda_c (\Phi - \tilde{c}) \overline{\rho u_i'' c''} \tilde{\varepsilon}_c / [\sigma_\varepsilon^2 + \tilde{c}(1 - \tilde{c})] \quad (5)$$

where $\lambda_c = 2$ and $\Phi = 0.5$ are model parameters and $\sigma_\varepsilon^2 = c''^2$ is the Favre variance of c . The model performance is shown in Fig. 3 which demonstrates that

eq. 5 satisfactorily captures the behaviour of $\overline{\rho u_i'' \varepsilon_c}$ without any change to the model parameters.

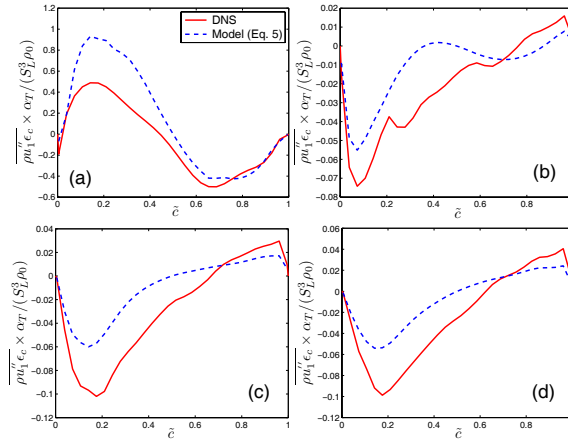


Fig. 3: Comparison of the model Eq.(5), prediction with $\overline{\rho u_i'' \varepsilon_c}$ obtained from DNS for (a) $Le = 0.34$, (b) $Le=0.8$, (c) $Le=1.0$ and (d) $Le=1.2$ flames.

Modelling of T_2

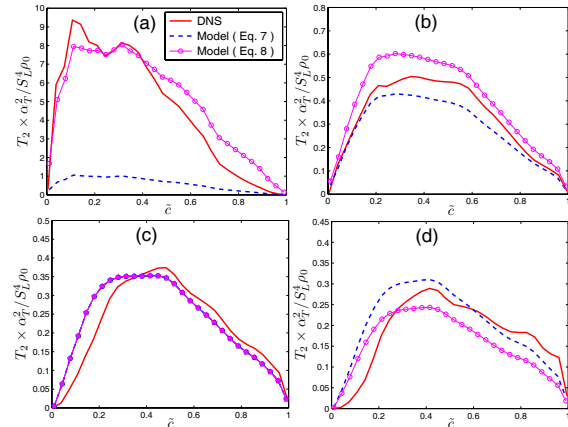


Fig. 4: Comparison of T_2 models predictions (Eqs. 7 and 8) with corresponding quantity obtained from DNS data for (a) $Le = 0.34$, (b) $Le = 0.8$, (c) $Le = 1.0$ and (d) $Le = 1.2$ flames.

The heat release related term can be written as [5-8] $T_2 = 2\overline{\rho \varepsilon_c (\nabla \cdot \vec{u})}$ for unity Lewis number flames. This term is given by Eq.(3c) for non-unity Le flames. The density gradients in Eq.(3) can be replaced by temperature gradients using the state equation appropriately. Thus, the correlation between ∇T and ∇c determines the behaviour of T_2 in response to Le . In the $Le < 1$ flames, these two gradients are positively correlated strongly compared to the $Le \geq 1$ flames. Thus, the magnitude of T_2 is large in $Le < 1$ flames as noted in Fig.2. If one uses the following scalings: $D \sim S_L \delta_{th} / Le$, $\dot{w} + \nabla \cdot (\rho \mathcal{N}c) \sim \rho_0 S_L / \delta_{th}$ and $\sqrt{c^{\prime 2} T^{\prime 2}} / \delta_{th} \delta_{th}$ for the correlation of the gradients ∇T and ∇c , then T_2 in Eq.(3c) scales as:

$$T_2 \sim O(\tau \cdot \rho_0 S_L \sqrt{c^{\prime 2} T^{\prime 2}} / \delta_{th} \delta_{th}) \quad (6)$$

Equation (6) suggests that T_2 will become increasingly strong with decreasing Le because the fluctuation of T is likely to be greater than the fluctuation of c in the $Le < 1$ flames because of weaker thermal diffusion rate compared to mass diffusion rate. In an earlier study [8], a simple model for T_2 in unity Le flames is proposed as

$$T_2 = 2C_{T_2} \tau \cdot S_L \overline{\rho \varepsilon_c} / \delta_{th} \quad (7)$$

where $C_{T_2} = B_{T_2}(1+Ka)^{-1/2}$ is the model parameter and B_{T_2} is a constant of order of unity but it depends on thermo-chemistry. The dilatation rate was scaled as $\nabla \cdot \vec{u} \sim \tau S_L / \delta_{th}$ for the above model [8] but for non-unity Le flames, the dilatation scales as [10] $\nabla \cdot \vec{u} \sim (\tau / Le^m)(S_L / \delta_{th})$, where $m > 0$ is of the order of unity. This scaling, indicates that the dilatation rate increases as Le decreases, which yields a model for T_2 as

$$T_2 = 2 \frac{1}{Le^n} \frac{\delta_{th}}{\delta_{th}} \sqrt{\frac{T^{\prime 2}}{c^{\prime 2}}} \frac{B_{T_2}}{(1+Ka_L)^{1/2}} \tau \frac{S_L}{\delta_{th}} \overline{\rho \varepsilon_c} \quad (8)$$

This model reverts to Eq. (7) for unity Le flames. The predictions of Eqs.(7) and (8) are compared to the DNS results in Fig.4. The values of B_{T_2} and n are taken to be about 2.0 and 0.88 respectively for all the flames in Table 1. Figure 4 indicates that Eq.(8) agrees well with the DNS data and Eq.(7) under predicts T_2 for the $Le \ll 1$ flames, while their predictions are the same for the unity Le flame.

Modelling of turbulence-scalar interaction term, T_3

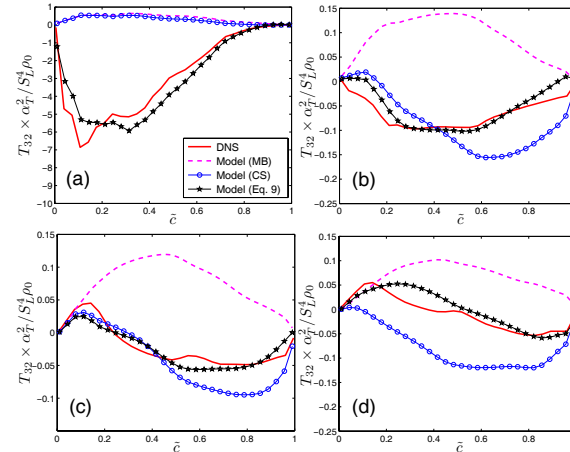


Fig. 5: Comparison of T_{32} models predictions (MB [3] and CS [7,8] models and Eq. 9) with corresponding quantity obtained from DNS data for (a) $Le = 0.34$, (b) $Le = 0.8$, (c) $Le = 1.0$ and (d) $Le = 1.2$ flames.

The influences of Le on the turbulence-scalar interaction have been studied in [10], which showed that strong heat release induced strain rate in small Le flames leads to a strong alignment of ∇c vector with the most extensive principal eigenvector of turbulent strain rate tensor as has been observed for unity Le flames [6, 7] with large Da . The investigation by Chakraborty *et al.* [10] also indicated that T_{32} (see Eq. 3d) is the leading order contributor to T_3 for all the Le cases considered here. Thus, T_{32} modelling of is the main focus here, while T_{31} and T_{33} modelling of will be addressed in

future investigation as Chakraborty *et al.* [10] suggested earlier models [3,7] satisfactorily predict the qualitative behaviours of T_{31} and T_{33} for flames with Le ranging from 0.34 to 1.2. Furthermore, earlier models [3, 7] for T_{32} were found to be inadequate for $Le \neq 1$ flames [10]. This is mainly because those models used a scaling for the strain rate induced by heat release ($a_{chem} \sim \tau S_L / \delta_L$) which is inadequate to account for differential diffusion effects for non-unity Le flames. A scaling for strain rate induced by chemical heat release is proposed here in the following manner: $a_{chem} \sim \tau f(Le) S_L / \delta_L$, where $f(Le)$ is taken to be $f(Le) = (1 - \tilde{c})^{\Phi(Le)} / Le^p$, with $p = 2.57$ and $\Phi(Le) = 0.2 + 1.5(1 - Le)$. Using this scaling and the earlier modelling strategy [3,7], one can obtain the following model for T_{32} in non-unity Le flames:

$$T_{32} = \bar{\rho}(\tilde{\epsilon} / \tilde{k}) [C_3^* - C_4^* \tau f(Le) Da_L^*] \tilde{\epsilon}_c \quad (9)$$

The model parameters C_3^* and C_4^* are taken to be 2.0 and $1.2(1 + Ka_L)^{-0.4}$ respectively. This model automatically degenerates to an earlier model [7, 8] for unity Le flames. Figure 5 compares the prediction of T_{32} model given by Eq.(9) with the DNS result and the values predicted by the earlier models from Refs. [3] and [8] (MB model[3]: $T_{32} = 0.9\bar{\rho}(\tilde{\epsilon} / \tilde{k})\tilde{\epsilon}_c$ and CS model [8] $T_{32} = \bar{\rho}(\tilde{\epsilon} / \tilde{k})[C_3 - C_4 \tau Da_L^*]\tilde{\epsilon}_c$ with $C_3 = 1.5$ and $C_4 = 1.1(1 + Ka_L)^{-0.4}$). For the $Le = 0.34$ flame the effects of above modifications are drastic and the model prediction is found to be in close agreement with the DNS results but the other models are unable to get even the sign correct. For the unity Le flame, the new model prediction is comparable to the model proposed in Refs. [7,8]. The difference between the new model and CS model in Fig.5c is because of the small difference in the values of C_3^* and C_4^* with C_3 and C_4 .

Modelling of reaction and dissipation terms, T_4 & D_2

Figure 6 shows the variations of $(T_4 - D_2)$ and $T_4^* = (T_4 + D_1 - D_2)$ across the flame brush. These two quantities are almost equal for all the flames. This implies that the molecular diffusion term D_1 is negligible compared to $(T_4 - D_2)$ and thus it can be eliminated from further consideration. The net contribution of $(T_4 - D_2)$ is observed to be negative in all the flames, implying that this contribution serves as sink for the evolution of the mean scalar dissipation rate. This is because of the predominant influence of the dissipation term, $-D_2$, which is determined by the correlation between the curvature and the dissipation rate N_c and the correlation between the displacement speed and the reaction progress variable gradient as has been noted in an earlier study [8]. Detailed analyses show that these observations equally apply for non-unity Le flames also. Mantel and Borghi [3] proposed a model for T_4^* as

$$T_4^* = -(2/3)\beta_1 \bar{\rho} \tilde{\epsilon}_c^2 (3/2 - C_{ec} S_L / \sqrt{\tilde{k}}) / [\tilde{c}(1 - \tilde{c})] \quad (10)$$

The predictions of this model with $\beta_1 = 6.5$ and $C_{ec} = 0.1$ are found to be close to the DNS results for all the flames as evident from Fig. 6. Since D_1 is negligible and furthermore it is a closed term, Chakraborty *et al.* [8] proposed a model for $(T_4 - D_2)$ as follows:

$$(T_4 - D_2) = -\beta_2 \bar{\rho} \tilde{\epsilon}_c^2 / [\tilde{c}(1 - \tilde{c})] \quad (11)$$

where $\beta_2 = 6.7$ is a model parameter for which the above model is realisable. Prediction of this model is also shown in Fig.6, which also is in good agreement with $(T_4 - D_2)$ for all the cases considered here.

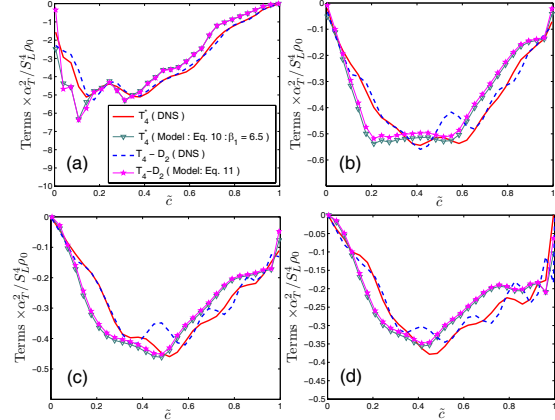


Fig. 6: Variations of $(T_4 - D_2)$ and $T_4^* = (T_4 + D_1 - D_2)$ across the flame brush along with model predictions for (a) $Le = 0.34$, (b) $Le = 0.8$, (c) $Le = 1.0$ and (d) $Le = 1.2$.

Interrelation between $\tilde{\epsilon}_T$ and $\tilde{\epsilon}_c$

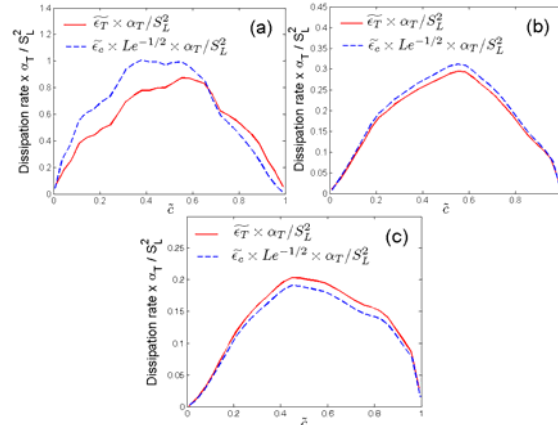


Fig. 7: Variations of the mean dissipation rates of temperature and the progress variable variance for (a) $Le = 0.34$, (b) $Le = 0.8$ and (c) $Le = 1.2$ flames.

It has been noted earlier, T and c are not identical in non-unity Le flames. Hence \tilde{c}^2 differs from \tilde{T}^2 and thus the scalar dissipation rate of non-dimensional temperature $\tilde{\epsilon}_T = \overline{\rho \alpha_T \nabla T^n \cdot \nabla T^n} / \bar{\rho}$ is required to close the transport equation for \tilde{T}^2 . One can follow the method discussed above using a transport equation for the temperature dissipation rate. Alternatively, one can use the scaling relations of the above two dissipation rates to obtain $\tilde{\epsilon}_T$. These two quantities can be scaled as $\tilde{\epsilon}_c \sim 1/t_c$ and $\tilde{\epsilon}_T \sim 1/t_T$ and the time scales are given by $t_c = \eta_c^2 / D$ and $t_T = \eta_{th}^2 / \alpha_T$ with η_{th} and η_c as the dissipation cut-off scales for T and c fields respectively. As both Prandtl number Pr and Schmidt number Sc are smaller than unity the dissipation length scales

(Obukov-Corrsin scale) for thermal and reaction progress variable fields η_{th} and η_c can be expressed as [16] $\eta_{th} = Pr^{0.75}/\eta$ and $\eta_c = Sc^{0.75}/\eta$, where η is Kolmogorov length scale. Thus, ratio of the above two dissipation rates yields $\tilde{\epsilon}_T \sim \tilde{\epsilon}_c Le^{-1/2}$. Figure 7 compares this relation using the DNS data and comparison is found to be satisfactory for the non-unity Lewis number flames.

Conclusions

Effects of Lewis number on scalar dissipation rate transport have been studied using three dimensional DNS data of freely propagating statistically planar flames under identical conditions of initial turbulent flow field. The combustion is simulated using a single irreversible reaction with global Lewis number ranging from 0.34 to 1.2. The stronger flame normal acceleration in $Le = 0.34$ flames leads to counter-gradient transport of turbulent flux of scalar dissipation rate whereas gradient transport is observed for the $Le=1.0$ and 1.2 flames. A model for the turbulent flux of scalar dissipation rate is proposed in terms of the turbulent scalar flux, $\overline{\rho u_i c''}$, which can predict both gradient and counter-gradient transport of the dissipation rate for all Le flames considered here. It has been found that the existing model [8] for unclosed term arising from density change T_2 in the dissipation rate transport equation significantly underpredict DNS values for the the $Le<1$ flames and the extent of this underprediction increases with decreasing Le . The scaling used for dilatation rate in the earlier model for T_2 does not account for the strengthening of dilatation rate due to enhanced burning at small values of Le . A new model for T_2 is proposed where strengthening (weakening) of dilatation rate effects for $Le<1$ ($Le>1$) flames in comparison to the unity Lewis number flame is explicitly accounted for. The Lewis number has significant influence on the interaction of turbulent velocity and scalar fields. It is observed that this interaction, denoted by T_3 in the $\tilde{\epsilon}_c$ transport equation, acts as a sink term in the $Le=0.34$ and 0.8 flames, whereas it is a source for a major portion of the flame brush before becoming a sink towards the burned gas side in $Le=1.0$ and 1.2 flames. This difference in behaviour originates because of the difference in the alignment of ∇c with local principal strain rates in different Lewis number flames. The existing models for the leading order component of the turbulence-scalar interaction T_{32} are found to be inadequate to capture the non-unity Le effects. A new model for T_{32} is proposed in this study where strengthening (weakening) of chemical heat release effects in the $Le<1$ ($Le>1$) flames in comparison to the unity Lewis number flame is explicitly taken into account. It is found that the existing model for the net contributions of chemical reaction and the molecular dissipation in the $\tilde{\epsilon}_c$ transport equation (i.e. (T_4-D_2)) satisfactorily predicts the corresponding quantity obtained from DNS data for all the different Le flames without any modification to the model

parameter. Although the functional form of the different modelling parameters given in this work are proposed in such a manner that they follow the asymptotic behaviour in relation to Damköhler and Karlovitz numbers, it is likely their numerical values need to be modified for higher values of turbulent Reynolds number. Thus, the sensitivity of the proposed model parameters in relation to turbulent Reynolds number needs to be investigated further using experimental data at high Reynolds number, where Damköhler and Karlovitz numbers can be altered independently for accurate estimation of the modelling constants. Moreover, the effects of detailed chemistry and global curvature are likely to augment some of the differential heat and mass diffusion rate effects which are not accounted for in this study. This will be addressed in future investigations.

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