Lai J, Alwazzan D, Chakraborty N.

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Turbulent scalar flux transport in head-on quenching of turbulent premixed flames: A Direct Numerical Simulations approach to assess models for Reynolds Averaged Navier Stokes simulations

Jiawei Lai¹, Dana Alwazzan¹, Nilanjan Chakraborty^{1,*}

¹School of Mechanical and Systems Engineering

University of Newcastle

Claremont Road, Newcastle

NE1 7RU, UK

Email: nilanjan.chakraborty@ncl.ac.uk

* Corresponding author

ABSTRACT

The statistical behaviour and the modelling of turbulent scalar flux transport have been analysed using a Direct Numerical Simulation (DNS) database of head-on quenching of statistically planar turbulent premixed flames by isothermal wall. A range of different values of Damköhler, Karlovitz numbers and Lewis numbers has been considered for this analysis. The magnitudes of the turbulent transport and mean velocity gradient terms in the turbulent scalar flux transport equation remain small in comparison to the pressure gradient, molecular dissipation and reaction-velocity fluctuation correlation terms in the turbulent scalar flux transport equation when the flame is away from the wall but the magnitudes of all these terms diminish and assume comparable values during flame quenching before vanishing altogether. It has been found that the existing models for the turbulent transport, pressure gradient, molecular dissipation and reaction-velocity fluctuation correlation terms in the turbulent scalar flux transport equation do not adequately address the respective behaviours extracted from DNS data in the near-wall region during flame quenching. Existing models for transport equation based closures of turbulent scalar flux have been modified in such a manner that these models provide satisfactory prediction both near to and away from the wall.

Keywords: Turbulent scalar flux, turbulent Reynolds number, Damköhler number, Karlovitz number, Reynolds Averaged Navier Stokes simulations

1. INTRODUCTION

Turbulent scalar flux is a quantity of fundamental interest in heat and mass transfer in the analysis of turbulent flows [1]. To date, most analyses [2-23] on statistical behaviour and modelling of turbulent scalar flux in turbulent reacting flows have been carried out for flows away from walls. The most commonly used turbulent scalar flux model assumes a gradient hypothesis [1] even though it is well-known [24,25] that the gradient transport does not sufficiently approximate the statistical variation of turbulent scalar flux [2-23] for both reacting and non-reacting flows. Furthermore, counter-gradient model has been reported based on theoretical [2], experimental [3,10,15] and computational [4-9,11-14,16-23] analyses. A counter-gradient transport is obtained when transport due to flame-normal acceleration dominates over the transport arising from turbulent velocity fluctuations [5-8,16-18,21-23]. By contrast, a gradient type transport is obtained when the transport due to turbulent velocity fluctuation overcomes that arising from flame normal acceleration [5-8,16-18,21-23]. Turbulent scalar flux can be closed by either an algebraic expression [1,2,5,9,11,12,14,18,20-24,26-30] or solving a modelled transport equation [13,17,20,24]. It is worth noting that the models based on Bray Moss Libby (BML) analysis [2] are strictly valid for infinitely fast chemistry (characterised by high values of Damköhler number given by $Da \gg 1$), where the probability density function of c can be approximated by a bimodal distribution with impulses at $c = 0$ and $c = 1$. The original BML based model expressions have been modified by Chakraborty and Cant [17,18,20] for low Damköhler number (i.e. $Da < 1$) combustion in the absence of the wall. To date, most models for turbulent scalar flux and the unclosed terms of its transport equation for reacting flows have been proposed for flows sufficiently away from the wall. The increasing demands for lightweight and micro-combustors make flame-wall interaction an inevitable event in these applications. It is necessary to have high-fidelity models for turbulent scalar flux in the near-wall region in order to accurately simulate the flame-wall

interaction. The influence of the wall on the statistical behaviours of turbulent scalar flux transport in turbulent reacting flows is yet to be analysed in detail. Furthermore, it is yet to be analysed if the scalar flux closures which were originally proposed for steady-state conditions can be applied for an intrinsically unsteady situation such as wall-induced flame quenching. This gap in existing literature is addressed here by analysing the performances of the closures of turbulent scalar flux and the terms of its transport equation in the context of Reynolds Averaged Navier Stokes (RANS) simulations of head-on quenching of turbulent premixed flames. A schematic diagram of head-on quenching of a statistically planar flame is shown in Fig. 1a which shows that the flame propagation direction is perpendicular to the inert isothermal wall in this configuration. For this purpose, a simple chemistry DNS database of head-on quenching of turbulent premixed flames by an isothermal wall for different values of Damköhler and Karlovitz numbers (i.e. Da and Ka) has been considered. Chakraborty and Cant [16-18] indicated that global Lewis number Le can have significant influences on statistical behaviour and modelling of turbulent scalar flux and the terms of its transport equation even when the flow remains away from the wall. Thus, all head-on quenching simulations in this analysis have been carried out for three different values of global Lewis number (i.e. $Le = 0.8, 1.0$ and 1.2).

An algebraic closure of turbulent scalar flux $\overline{\rho u_i'' c''}$ with near-wall modification has been addressed elsewhere [31] and thus are not repeated here. Thus, the modelling of the unclosed terms of the transport equation of $\overline{\rho u_i'' c''}$ will be discussed in this paper. The transport equation based closure of turbulent scalar flux has received limited attention in combustion literature [17,20]. However, in principle, a transport equation based closure accounts for all the necessary physical mechanisms, which can affect the statistical behaviour of turbulent scalar flux. Moreover, it is often necessary to solve transport equations of turbulent scalar flux

components in the context of a second moment closure approach [32], and interested readers are referred to Lindstedt and Vaos [32] and Lindstedt [33] for more detailed discussion on this.

The main objectives of the present analysis are:

- (a) To demonstrate the near-wall behaviour of the unclosed terms of the transport equation of the turbulent scalar flux of reaction progress variable.
- (b) To propose models for the near-wall behaviour of the terms of the turbulent scalar flux transport equation.

The rest of the paper will be organised as follows. The mathematical background and numerical implementation pertaining to this analysis are presented in the next two sections. Following that, results are presented and subsequently discussed. The main findings will be summarised, and conclusions will be drawn in the final section of this paper.

2. MATHEMATICAL BACKGROUND

In the interest of computational economy, the chemical mechanism is simplified here by a single step Arrhenius type chemical reaction (i.e. *Reactants* $\rightarrow$ *Products*) because detailed chemistry three-dimensional DNS simulations are still prohibitively expensive to conduct an extensive parametric analysis as carried out in this analysis [34]. In premixed flames the species field is often characterised by a reaction progress variable c which is defined based on a suitable reactant mass fraction Y_R as:

$$c = \frac{Y_{R0} - Y_R}{Y_{R0} - Y_{R\infty}} \quad (1)$$

where the subscripts 0 and ∞ refer to values in unburned reactants and fully burned products respectively. The transport equation of c takes the following form:

$$\frac{\partial(\rho c)}{\partial t} + \frac{\partial(\rho u_j c)}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\rho D \frac{\partial c}{\partial x_j} \right) + \dot{w} \quad (2)$$

where $\rho, u_j, \dot{w}$ and D are the density, j^{th} component of velocity, reaction rate and progress variable diffusivity respectively. On Reynolds averaging eq. 2 one obtains:

$$\frac{\partial(\bar{\rho}\tilde{c})}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_j\tilde{c})}{\partial x_j} = \overline{\frac{\partial}{\partial x_j}\left(\rho D \frac{\partial c}{\partial x_j}\right)} + \bar{\dot{w}} - \frac{\partial(\overline{\rho u_j'' c''})}{\partial x_j} \quad (3)$$

where $\bar{q}, \tilde{q} = \overline{\rho q} / \bar{\rho}, q' = q - \bar{q}$ and $q'' = q - \tilde{q}$ are the Reynolds averaged, Favre averaged Reynolds fluctuation and Favre fluctuation of a general quantity q respectively. The last two terms on the right-hand side of eq. 3 are unclosed and need modelling. The molecular diffusion term $\overline{\nabla \cdot (\rho D \nabla c)}$ can be neglected in comparison to the value of $\nabla \cdot \overline{\rho \vec{u}'' c''}$ for large values of turbulent Reynolds number. The reaction-diffusion imbalance term $\bar{\dot{w}} + \overline{\nabla \cdot (\rho D \nabla c)}$ can be modelled as $\overline{(\rho S_d)}_s \Sigma_{gen}$ in the context of FSD based closure, where $S_d = (Dc/Dt)/|\nabla c|$ is the displacement speed, $\Sigma_{gen} = |\nabla c|$ is the generalised FSD [35] and $\overline{(q)}_s = \overline{q|\nabla c|}/\Sigma_{gen}$ indicates the surface averaged value of a general variable q . The modelling of the last term on the right hand side of eq. 3 represents turbulent transport of reaction progress variable and its modelling depends on the closure of turbulent scalar flux components $\overline{\rho u_j'' c''}$. The quantity $\overline{\rho u_j'' c''}$ is often closed in terms of an algebraic expression [1,2,5,9,11,12,14,18,20-24,26-30] or a modelled transport equation for $\overline{\rho u_j'' c''}$ is solved [13,17,20,24]. The most conventional algebraic model for $\overline{\rho u_j'' c''}$ uses the gradient hypothesis in the following manner:

$$\overline{\rho u_j'' c''} = -\bar{\rho} D_t \frac{\partial \tilde{c}}{\partial x_j} \quad (4)$$

where D_t is the eddy diffusivity. According to the Bray-Moss-Libby (BML) analysis [2] the probability density function (pdf) of c is assumed to follow a bimodal distribution with impulses at $c = 0$ and $c = 1.0$, which leads to:

$$\overline{\rho u_j'' c''} = \bar{\rho} \left[\overline{(u_j)}_P - \overline{(u_j)}_R \right] \tilde{c}(1 - \tilde{c}) + O(\gamma_c) \quad (5)$$

where $\overline{(u_j)}_P$ and $\overline{(u_j)}_R$ are the j^{th} components of conditional mean velocity in products and reactants respectively and the last term on right-hand side arises due to the contribution of the reacting mixture (i.e. from $0 < c < 1$). The weight of the contribution arising from the interior of the flame (i.e. from $0 < c < 1$) is given by γ_c . The contribution of $O(\gamma_c)$ remains negligible for high Damköhler number (i.e. $Da \gg 1$) combustion.

The exact transport equation of $\overline{\rho u_i'' c''}$ can be derived based on momentum and reaction progress variable transport equations as [13,17,20,24]:

$$\begin{aligned}
& \frac{\partial(\bar{\rho} \widetilde{u_i'' c''})}{\partial t} + \frac{\partial(\bar{\rho} \widetilde{u_j} \widetilde{u_i'' c''})}{\partial x_j} \\
&= \underbrace{-\frac{\partial \overline{\rho u_i'' u_j'' c''}}{\partial x_j}}_{T_1} \underbrace{-\overline{\rho u_i'' u_j''} \frac{\partial \tilde{c}}{\partial x_j}}_{T_2} \underbrace{-\overline{\rho u_j'' c''} \frac{\partial \tilde{u}_i}{\partial x_j}}_{T_3} \underbrace{-\overline{c''} \frac{\partial \bar{P}}{\partial x_i}}_{T_4} \underbrace{-\overline{c''} \frac{\partial P'}{\partial x_i}}_{T_5} \\
&+ \underbrace{\left[u_i'' \frac{\partial}{\partial x_k} \left(\rho D \frac{\partial c}{\partial x_k} \right) \right]}_{T_6} + \underbrace{\left[c'' \frac{\partial \tau_{ik}}{\partial x_k} \right]}_{T_7} + \underbrace{\overline{u_i'' \dot{w}}}_{T_8}
\end{aligned} \tag{6}$$

where P is the pressure, $\tau_{ik} = \mu[\partial u_i / \partial x_k + \partial u_k / \partial x_i] - (2\mu/3)\delta_{ik}(\partial u_l / \partial x_l)$ is the component of viscous stress in tensor. The terms on the left-hand side are the transient and mean advection terms. The term T_1 represents turbulent transport of $\widetilde{u_i'' c''}$, whereas T_2 and T_3 represent turbulent scalar flux transport due to mean scalar and velocity gradients respectively. The terms T_4 and T_5 are responsible for turbulent scalar flux transport by mean and fluctuating pressure gradients respectively. The terms T_6 and T_7 originate due to mass diffusion and viscous stress respectively, and these terms act to reduce the magnitude of $\widetilde{u_i'' c''}$ irrespective of the nature of scalar flux transport. Thus, these terms are often referred to dissipation terms. The last term on the right-hand side T_8 originates from the correlation between reaction rate

and reaction progress variable fluctuations. The terms T_1, T_4, T_5, T_6, T_7 and T_8 are the unclosed terms and need modelling, whereas the terms T_2 and T_3 are closed because modelled transport equations for $\overline{\rho u_i'' u_j''}$ and $\overline{\rho u_j'' c''}$ are solved in the context of second-moment closure. The statistical behaviour and modelling of T_1, T_4, T_5, T_6, T_7 and T_8 will be discussed in Section 4.

3. NUMERICAL IMPLEMENTATION

A compressible DNS code SENGa [36] has been used to carry out three-dimensional DNS simulations of head-on quenching of premixed turbulent flames, and in this framework the conservation equations of mass, momentum, energy and reaction progress variable are solved in the non-dimensional form in a coupled manner. The simulations domain has been taken to be $70.6\delta_Z \times 35.2\delta_Z \times 35.2\delta_Z$ (where $\delta_Z = \alpha_{T_0}/S_L$ is the Zel'dovich flame thickness with α_{T_0} and S_L being the thermal diffusivity of unburned gas and unstrained laminar burning velocity respectively) with the largest side aligned with the mean direction of flame propagation (i.e. -ve x_1 -direction here). The simulation domain is discretised using a uniform Cartesian grid of size $512 \times 256 \times 256$, which ensures 10 grid points across the thermal flame thickness $\delta_{th} = (T_{ad} - T_0)/\text{Max} |\nabla \hat{T}|_L$ where T_{ad}, T_0 and $\hat{T}$ are the adiabatic flame, unburned gas and instantaneous temperature respectively. A no-slip isothermal inert wall with temperature $T_w = T_0$ is specified for the left-hand side boundary in the x_1 -direction, and the boundary opposite to the wall is considered to be partially non-reflecting. The wall normal mass flux is considered to be zero, which can be written as $(\partial c / \partial x_1)_{x_1=0} = 0$ at the wall. The boundaries in x_2 and x_3 directions are considered to be periodic. The schematic diagram of the domain is shown in Fig. 1b. A 10th order central difference scheme is used for numerical spatial differentiation for the internal grid points but the order of differentiation gradually drops to a one-sided 2nd order

scheme at the non-periodic boundaries. A low storage 3rd order Runge-Kutta scheme [37] has been used for explicit time marching.

A steady unstrained planar laminar premixed flame solution is used to initialise the reactive field. The flame is initially placed away from the wall so that $T = (\hat{T} - T_0)/(T_{ad} - T_0) = 0.9$ isosurface remains at a distance $20\delta_z$ away from the wall. The distance ensures that the flame gets enough time to evolve before interacting with the wall. The velocity field is initialised using a homogeneous isotropic field of turbulent velocity fluctuations, which is generated using a pseudo-spectral method [38] following the Batchelor-Townsend Spectrum [39], but the velocity components at the wall u_1 , u_2 and u_3 are specified to be zero to ensure no-slip condition. This field is allowed to evolve for an initial eddy turn-over time before interacting with the flame.

The initial values of normalised root-mean-square (rms) turbulent velocity fluctuation u'/S_L , the ratio of longitudinal integral length scale to thermal flame thickness L_{11}/δ_{th} for the turbulent velocity field away from the wall are listed in Table 1 along with the corresponding values of Damköhler number $Da = L_{11}S_L/\delta_{th}u'$, Karlovitz number $Ka = (u'/S_L)^{3/2}(L_{11}/\delta_{th})^{-1/2}$ and turbulent Reynolds number based on L_{11} (i.e. $Re_t = \rho_0 u' L_{11}/\mu_0$). One will get an increase in the numerical value of Re_t by a factor of almost 2.35 if the integral length scale $l_T = \tilde{k}^3/\tilde{\epsilon}$ is used. The turbulent Reynolds number values used here are comparable to the values used in the previous analyses [5-23] which concentrated on the turbulent scalar flux modelling in turbulent premixed flames. It can be seen from Table 1 that the cases A, C and E (B, C and D) have same values of Da (Ka). Three different global Lewis numbers (i.e. $Le = 0.8, 1.0$ and 1.2) have been considered for each set of turbulence parameters considered here. Standard values are chosen for Prandtl number Pr and ratio of specific heats

γ (i.e. $Pr = 0.7$ and $\gamma = 1.4$). For the present analysis, both the heat release parameter $\tau = (T_{ad} - T_0)/T_0$, and Zel'dovich number $\beta = E_{ac}(T_{ad} - T_0)/RT_{ad}^2$ are taken to be 6.0 (i.e. $\tau = 6.0$ and $\beta = 6.0$). The values $\beta = 6.0$ and $\tau = 6.0$ are representative of an iso-octane-air mixture with unburned gas temperature $T_0 \approx 325.0K$ and equivalence ratio of 1.10 under atmospheric pressure. The gaseous mixture is assumed to follow the ideal gas laws, and the flame Mach number $Ma = S_L/\sqrt{\gamma RT_0}$ is taken to be 0.014 due to small Mach number in most engineering combustion processes [40]. The simulations for turbulent cases have been carried out until a time when the maximum and minimum values of wall heat flux become identical values following the flame quenching. The simulation time remains different for different cases, but the simulations for all cases were continued for $t \geq 12\delta_Z/S_L$ where $12\delta_Z/S_L$ corresponds to 21, 30, 21, 15 and 21 initial eddy turn-over times (i.e. $t_e = L_{11}/u'$) for cases A-E respectively. The non-dimensional grid spacing next to the wall $y^+ = u_\tau \Delta x/\nu$ remains smaller than unity for all turbulent cases (the maximum value of y^+ has been found to be 0.93 during the course of the simulation), where $u_\tau = \sqrt{\tau_w/\rho}$, τ_w and ν are the friction velocity, mean wall shear stress, and kinematic viscosity respectively. For $y^+ = u_\tau \Delta x/\nu \approx 0.93$, the minimum normalised wall normal distance $u_\tau x_1/\nu$ of $T = (\hat{T} - T_0)/(T_{ad} - T_0) = 0.9$ isosurface has been found to be about 15.0 for the quenching flames considered here.

For the purpose of extracting Reynolds/Favre averaged quantities the DNS data has been ensemble averaged on the transverse plane (i.e. x_2 and x_3 direction as these are statistically homogeneous directions in this configuration) at a given x_1 location at a given instant of time. The statistical convergence of Reynolds/Favre averaged quantities has been assessed by comparing the values obtained based on the full available sample size in the transverse directions (i.e. x_2 - x_3 directions) at a given x_1 location with the corresponding values evaluated using the distinct half of the available samples in the transverse directions, and a satisfactory

level of agreement has been found. In the next section, the results based on the full sample size in $x_2 - x_3$ directions will be presented for the sake of conciseness.

4. RESULTS & DISCUSSION

4.1 Global features of flame-wall interaction

The distributions of reaction progress variable c , non-dimensional temperature $T = (\hat{T} - T_0)/(T_{ad} - T_0)$ and non-dimensional reaction rate of reaction progress variable $\dot{w} \times \delta_Z / \rho_0 S_L$ in the central $x_1 - x_3$ plane for $Le = 0.8, 1.0$ and 1.2 are shown in Fig. 1c for case E. For unity Lewis number flames, c and T are identical to each other under adiabatic low Mach number conditions. This can be observed when the flame is away from the wall prior to the flame quenching. However, the adiabatic condition is not maintained in the case of isothermal boundary condition, and the equality between c and T does not hold during flame quenching. In the non-unity Lewis number flames the equality between c and T does not hold even when the flame is away from the wall. The regions with $T > c$ in the $Le = 0.8$ flame are associated with the regions where the flame surface is convex towards the reactants whereas $T < c$ are associated with flame surface concave to the reactants. Just the opposite behaviour has been observed for the $Le = 1.2$ flame and thus $T > c$ ($T < c$) is associated with the flame wrinkles which are concave (convex) to the reactants. This behaviour is consistent with several previous findings [41-44]. Figure 1c further suggests that flame starts to interact with the wall and quenching initiates at an earlier time in the case of $Le = 0.8$ ($Le = 1.0$) than in the $Le = 1.0$ ($Le = 1.2$) turbulent cases because of faster flame propagation for flames with smaller values of Lewis number. Faster diffusion of reactants into the reaction zone than the thermal diffusion rate out of it gives rise to simultaneous presence of high reactant concentration and high temperature, which leads to faster flame propagation in the $Le < 1$ flames than the corresponding unity Lewis number flame. Just the opposite mechanism gives rise smaller rate

of flame propagation and burning in turbulent $Le < 1$ flames than the corresponding turbulent unity Lewis number flame. Fast flame propagation and earlier initiation of flame quenching for small Lewis number flames can be seen from the normalised turbulent flame speed S_T/S_L (where $S_T = (\rho_0 A_p)^{-1} \int_V \dot{w} dV$, and A_p is the projected area in the direction of flame propagation), and normalised flame surface area A_T/A_L (where flame surface area has been evaluated here using the volume integral $A = \int_V |\nabla c| dV$, and turbulent and laminar values are shown with subscripts T and L respectively) values reported in Table 2, which also shows that the rate of flame propagation is faster for higher values of $u'/S_L \sim Re_t^{1/4} Ka^{1/2} \sim Re_t^{1/2} Da^{-1/2}$ when the flame is away from the wall and flame quenching initiates at an earlier time instant for higher values of u'/S_L . The reactants diffuse into the reaction zone at a faster rate than the rate of thermal diffusion out of it in the case of $Le < 1$, which in turn leads to simultaneous strong focusing of reactants and defocusing of heat in the positively stretched zones. This gives rise to simultaneous occurrence of high reactant concentration and temperature in positively stretched zones in turbulent $Le < 1$ flames, which augments the rate of burning, magnitude of dilatation rate and thereby strengthens the flame normal acceleration in comparison to unity Lewis number flames with statistically similar unburned gas turbulence (see e.g. [18] and references therein). By contrast, thermal diffusion rate supersedes the mass diffusion rate in $Le > 1$ flames and thus a combination of simultaneous strong defocusing of heat and weak focusing of reactants in the positively stretched zones leads to the weakening of the rate of burning, magnitude of dilatation rate and flame normal acceleration in comparison to unity Lewis number flames with statistically similar unburned gas turbulence. Interested readers are referred to Lai and Chakraborty [44] for further discussion on Lewis number effects on wall heat flux and flame wrinkling in the current configuration.

4.2 Statistical behaviour of turbulent scalar flux $\overline{\rho u_1'' c''}$

The only non-zero scalar flux component is $\overline{\rho u_1'' c''}/\rho_0 S_L$ in the present configuration. The variations of $\tilde{c}$, $\overline{\rho u_1'' c''}/\rho_0 S_L$ and $\overline{\rho u_1'' c''} \times (\partial \tilde{c}/\partial x_1) \times \delta_z/\rho_0 S_L$ with x_1/δ_z at three time instants $t = 2 \delta_z/S_L$, $6 \delta_z/S_L$ and $10 \delta_z/S_L$ are shown in Figs. 2, 3 and 4 respectively for cases A, C and E. Cases B and D are not shown for the sake of conciseness because of their qualitative similarities with cases A and E respectively. It is discussed in several previous analyses [5,11, 16-18] that the statistical behaviour of turbulent scalar flux is determined by the Bray number $N_B \propto \tau S_L/u'$. As cases B and A (D and E) have similar Bray number values due to similar u'/S_L , these cases show statistically similar turbulent scalar flux behaviour. The time instants $t = 2 \delta_z/S_L$, $6 \delta_z/S_L$ and $10 \delta_z/S_L$ are carefully chosen so that different stages (i.e. from flame being away from the wall to flame-wall interaction to flame quenching) can be exemplarily demonstrated for all cases considered here. The temporal evolutions of the maximum, mean and minimum values of non-dimensional wall heat flux $\Phi = |q_w|/[\rho_0 S_L C_p (T_{ad} - T_0)]$ (where q_w is the wall heat flux) are shown in Fig. 2b. It can be seen from Fig. 2b that quenching started at the last time instant (i.e. $t = 10 \delta_z/S_L$) shown here for case A with $Le = 1.2$ which shows the slowest propagation rate towards the wall among the cases considered here. The statistical behaviour of the wall heat flux is discussed elsewhere [44] and thus are not repeated here.

A comparison between Figs. 2a and 3 reveals that $\overline{\rho u_1'' c''}/\rho_0 S_L$ assumes predominantly positive values within the flame brush and its magnitude decreases with time as the quenching progresses. As the wall normal mass flux is zero, the value of $\tilde{c}$ increases at the wall (i.e. $x_1/\delta_z = 0$) subsequent to flame quenching during flame-wall interaction. A comparison between Figs. 2a and 3 reveals that both $\overline{\rho u_1'' c''}$ and $\partial \tilde{c}/\partial x_1$ are expected to show same signs

for the major part of the flame brush suggesting a predominance of counter-gradient transport (because the gradient and flux are expected to be of opposite sign for gradient transport according to eq. 4). This behaviour can further be substantiated from the behaviour of $\overline{\rho u_1'' c''} \times (\partial \tilde{c} / \partial x_1)$, which assumes a positive (negative) value for counter-gradient (gradient) transport. It can be seen from Fig. 4 that $\overline{\rho u_1'' c''} \times (\partial \tilde{c} / \partial x_1)$ predominantly assumes positive values suggesting a counter-gradient transport. However, some local negative values of $\overline{\rho u_1'' c''} \times (\partial \tilde{c} / \partial x_1)$ can be discerned in cases C and E, indicating localised presence of gradient type of transport in these cases. Several previous analyses [5-8,16-18,20] indicated that a counter-gradient transport is obtained when the flame normal acceleration significantly overcomes the transport due to turbulent velocity fluctuations and *vice versa*. This can further be elucidated by examining eq. 5 which suggests that a counter-gradient (gradient) transport is obtained for $\overline{(u_j)_P} > \overline{(u_j)_R}$ ($\overline{(u_j)_P} < \overline{(u_j)_R}$). Veynante *et al.* [5] modelled $\overline{(u_j)_P} - \overline{(u_j)_R}$ as:

$$\overline{(u_j)_P} - \overline{(u_j)_R} = [-\alpha_E u' + \tau S_L] \quad (7)$$

where α_E is an appropriate efficiency function [5]. Equation 7 leads to a non-dimensional number known as the Bray number N_B which is proportional to $\tau S_L / u'$ (i.e. $N_B \propto \tau S_L / u'$) [5] so that a counter-gradient (gradient) transport is obtained for $N_B \gg 1$ ($N_B \ll 1$). This indicates that the effects of gradient transport are expected to be stronger in case E (case C) than case C (case A). By contrast, case A (case C) is expected to show stronger counter-gradient transport than case C (case E). These expectations are consistent with the observations made from Fig. 4, which shows greater extent of gradient transport for cases C and E than in case A. Furthermore, the gradient transport is predominant towards the unburned gas side of the flame brush where the effects of flame normal acceleration due to thermal expansion arising from chemical heat release are weak. The spatial distributions of non-dimensional local rms turbulent velocity fluctuation $u' / S_L = \sqrt{2\tilde{k}/3} / S_L$ and the non-dimensional local integral

length scale where $l_T = (\tilde{k}^{3/2}/\tilde{\epsilon})/\delta_{th}$ are shown in Fig. 5a. It can be seen from Fig. 5a that the magnitudes of $\sqrt{2\tilde{k}/3}/S_L$ and $l_T/\delta_{th} = (\tilde{k}^{3/2}/\tilde{\epsilon})/\delta_{th}$ decrease with time but these values remain non-negligible for the time instants shown here so that these snapshots capture different stages of flame movement (i.e. from away from the wall to flame-wall interaction to flame quenching). Furthermore, a comparison between Figs. 2a and 5a reveals that relatively high values of $\sqrt{2\tilde{k}/3}/S_L$ and $l_T/\delta_{th} = (\tilde{k}^{3/2}/\tilde{\epsilon})/\delta_{th}$ are obtained ahead of the flame but they decrease across the flame brush and also in the vicinity of the isothermal inert wall. A combination of high values of $\sqrt{2\tilde{k}/3}$ and weak effects of heat release and flame normal acceleration at the leading edge of the flame brush gives rise to a gradient-type transport in cases C and E.

It is possible to define local Karlovitz and Damköhler numbers (i.e. Ka_L and Da_L respectively) in terms of local turbulent kinetic energy and its dissipation rate as: $Ka_L = (\tilde{\epsilon}\delta_{th})^{1/2} S_L^{-3/2}$ and $Da_L = \tilde{k}S_L(\tilde{\epsilon}\delta_{th})^{-1}$. The spatial variations of Ka_L and Da_L in the wall normal direction are shown in Fig. 5b. It can be seen from Fig. 5b that both Ka_L and Da_L assume high values in the unburned gas, and Ka_L also exhibits high values in the near-wall region when the flame is away from the wall, whereas $Da_L = \tilde{k}S_L(\tilde{\epsilon}\delta_{th})^{-1}$ decays towards the wall and becomes identically zero at the wall due to $\tilde{k} = 0$. The magnitudes of Da_L and Ka_L decrease with time due to the decay of turbulence, and this is particularly prevalent as the head-on quenching progresses because of increased probability of finding burned gas (where both $\tilde{k}$ and $\tilde{\epsilon}$ decay significantly) at the advanced stages of flame quenching (see Fig.1). At the advanced stages of flame quenching, the values of Ka_L and Da_L remain of the order of unity, especially in the near-wall region. However, cases C and E exhibit $Ka_L > 1.0$ in the near-wall region and also for $Le \leq 1.0$ in case A. The local turbulent Reynolds number Re_{tL} can be estimated as

$Re_{tL} \sim Da_L^2 Ka_L^2$ and thus Re_{tL} is also expected to be of the order of unity especially in the near-wall region at the advanced stages of flame quenching. This suggests that near-wall dynamics is dominated by viscous action at the advanced stages of flame quenching due to the decay of turbulence in this configuration. Thus, in the current configuration setup, the final stage of head-on quenching takes place under weak turbulence, and thus models need to perform satisfactorily in relatively strong turbulent conditions, when the flame is away from the wall, but they also are required to perform under decayed turbulence during advanced stages of flame quenching.

A comparison between different Lewis number cases reveal that the cases C and E exhibit greater extent of gradient transport for $Le = 0.8$ than for $Le = 1.0$ and 1.2 cases. It can be seen from Table 2 that the rate of flame propagation and the extent of flame wrinkling increase with decreasing Le and increasing u'/S_L , and it also indicates that S_T/S_L increases significantly with decreasing Le and increasing u'/S_L when the flame is away from the wall. However, faster flame propagation brings the flame wrinkles closer to the wall at earlier time instant for the $Le = 0.8$ case than in the corresponding $Le = 1.0$ and 1.2 cases. Thus, at a given time instant the $Le = 0.8$ case remains at a more advanced stage of flame quenching than the corresponding cases with higher values of Le . Thus, smaller values of A_T/A_L and S_T/S_L are obtained for the $Le = 0.8$ case at later times (i.e. $t \geq 4\delta_Z/S_L$) than in the corresponding cases with higher values of Le . As the effects of quenching set in by $t = 6\delta_Z/S_L$ in cases C and E with $Le = 0.8$, the effects of turbulence dominate over heat release to give rise to a gradient transport. However, the effects of flame quenching are comparatively less prominent in the $Le = 1.0$ and 1.2 cases, and thus relatively stronger influences of heat release overwhelm the effects of turbulence to result in a counter-gradient transport for $t \leq 6\delta_Z/S_L$.

4.3 Statistical behaviours of the terms in turbulent scalar flux transport equation

The variations of $T_1 - T_8$ for the $\overline{\rho u_1'' c''}$ transport equation with normalised wall normal distance x_1/δ_Z (shown in linear scale for the sake of better clarity) for cases A, C and E are shown in Fig. 6 for different time instants. The positive contributions in Fig. 6 act to promote a counter-gradient transport, whereas negative contributions tend to induce a gradient transport. It can be seen from Fig. 6 that the reaction contribution T_8 assumes predominantly positive values, whereas both T_6 and T_7 exhibit negative values at all times. The pressure gradient terms T_4 and T_5 play important roles in the transport of $\overline{\rho u_1'' c''}$ for all cases when the flame is away from the wall. The mean pressure gradient term T_4 assumes a positive value for the major part of the flame brush although local negative values of T_4 are also obtained within the flame brush when the flame is away from the wall. The fluctuating pressure gradient term T_5 also exhibits both positive and negative values within the flame brush. The contributions of T_2 and T_3 remain negative, whereas the turbulent transport term T_1 exhibits both positive and negative values. The relative magnitudes of T_1, T_2 and T_3 in comparison to the pressure gradient terms T_4 and T_5 decrease with increasing Re_t (i.e. from case A to case E). The magnitudes of $T_1 - T_8$ decrease considerably as the quenching progresses and they eventually vanish altogether.

The terms $T_1 - T_8$ can be scaled in the following manner [20]:

$$\begin{aligned}
 T_1 &\sim (\rho_0 S_L^2 / \delta_{th}) (\overline{\rho u_1'' c''} / \rho_0 S_L)^2 Da^{-0.5} Re_t^{-0.5}; T_2 \sim (\rho_0 S_L^2 / \delta_{th}) Da^{-1.5} Re_t^{0.5}; \\
 T_3 &\sim (\rho_0 S_L^2 / \delta_{th}) (\overline{\rho u_1'' c''} / \rho_0 S_L) (U_{ref} / S_L) Da^{-0.5} Re_t^{-0.5}; T_4 \sim (\rho_0 S_L^2 / \delta_{th}) Da^{-1.5} Re_t^{0.5}; \quad (8) \\
 T_5 &\sim (\rho_0 S_L^2 / \delta_{th}) (\overline{\rho u_1'' c''} / \rho_0 S_L)^2; T_6 \sim (\rho_0 S_L^2 / \delta_{th}) (\overline{\rho u_1'' c''} / \rho_0 S_L); \\
 T_7 &\sim (\rho_0 S_L^2 / \delta_{th}) (\overline{\rho u_1'' c''} / \rho_0 S_L) \text{ and } T_8 \sim (\rho_0 S_L^2 / \delta_{th}) (\overline{\rho u_1'' c''} / \rho_0 S_L)
 \end{aligned}$$

Here the gradients of the mean quantities are scaled using l and the quantities $\overline{\rho u_1'' u_1'' c''}$ and $\overline{\rho u_1'' u_1''}$ are scaled with respect to $(\overline{\rho u_1'' c''})^2 / \rho_0$ and $\rho_0 u'^2$ respectively. The mean pressure gradient can be taken to scale as $\partial \bar{P} / \partial x_1 \sim \partial (\overline{\rho u_1'' u_1''}) / \partial x_1$ for flows with u' either greater than or comparable to $\tilde{u}_1$, as in the cases considered here. In terms $T_5 - T_8$ the scalings of the key quantities may be taken as $\partial P' / \partial x_1 \sim (\rho u_1'' c'')^2 / \rho_0 \delta_{th}$, $u_1'' \sim \rho u_1'' c'' / \rho_0$ and $\partial \tau_{ik} / \partial x_k \sim (\rho u_1'' c'') (S_L / \delta_{th})$. The molecular diffusion rate and reaction rate in T_7 and T_8 have been scaled with respect to $\rho_0 S_L / \delta_{th}$ (i.e. $\dot{w} \sim \rho_0 S_L / \delta_{th}$ and $\nabla \cdot (\rho D \nabla c) \sim \rho_0 S_L / \delta_{th}$). The scaling estimates given by eq. 8 indicate that the terms $T_2, T_4 - T_8$ are expected to be the leading order contributors for $Da < 1$, whereas the contributions of T_1 and T_3 are expected to become progressively less important with increasing Re_t . The terms T_2 and T_3 are closed in the context of second-moment closure, and thus the modelling of T_1 and T_4 to T_8 will be discussed next.

4.4 Modelling of the turbulent transport term T_1

The turbulent transport term is given by: $T_1 = \partial (\overline{\rho u_j'' u_i'' c''}) / \partial x_j$, and therefore modelling of this term depends on $\overline{\rho u_j'' u_i'' c''}$. The model (referred to as the TDH model) by Daly and Harlow [45] is one of the widely used models for $\overline{\rho u_j'' u_i'' c''}$ closure for passive scalars:

$$\overline{\rho u_i'' u_j'' c''} = -C_{CS} \frac{\tilde{k}}{\tilde{\epsilon}} \overline{\rho u_j'' u_k''} \frac{\partial (\overline{\rho u_i'' c''} / \bar{\rho})}{\partial x_k} \quad (9)$$

where $\tilde{\epsilon} = \overline{\mu (\partial u_i'' / \partial x_j) (\partial u_i'' / \partial x_j)} / \bar{\rho}$ is the dissipation rate of kinetic energy $\tilde{k}$, and $C_{CS} \approx 0.22$ is the model constant. The predictions of the TDH model are compared to $\overline{\rho u_1'' u_1'' c''}$ extracted from DNS data in Fig. 7. The TDH model fails to capture the quantitative and qualitative behaviour of the DNS data, for cases A-C. However, for high values of

$u'/S_L \sim Re_t^{\frac{1}{4}} Ka^{\frac{1}{2}} \sim Re_t^{\frac{1}{2}} Da^{-\frac{1}{2}}$ (e.g. cases D and E) the TDH model exhibits slightly improved agreement with DNS data at $t \leq 6 \delta_Z/S_L$ but this model fails to predict the near-wall behaviour of $\overline{\rho u_1'' u_1'' c''}$ at $t \geq 8 \delta_Z/S_L$. The TDH models is proposed for non-reacting flow based on gradient hypothesis, and it does not take into account for the effect of chemical reaction. According to the BML analysis (i.e. subject to the assumption of bimodal probability density function of c (i.e. $P(c)$) with impulses at $c = 0$ and $c = 1$) the Favre-average velocity component takes the following form: $\tilde{u}_j = \overline{(u_j)}_P \tilde{c} + (1 - \tilde{c}) \overline{(u_j)}_R + O(1/Da)$, which once used in $\overline{\rho u_i'' u_j'' c''} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_0^1 \rho(u_i - u_i)(u_j - \tilde{u}_j) P(u_i, u_j, c) du_i du_j dc$ yields [20,46]:

$$\begin{aligned} \overline{\rho u_1'' u_1'' c''} \approx \bar{\rho} [\overline{(u_1)}_P - \overline{(u_1)}_R]^2 \tilde{c}(1 - \tilde{c})(1 - 2\tilde{c}) - \bar{\rho} \overline{(u_1' u_1')}_R \tilde{c}(1 - \tilde{c}) + \bar{\rho} \overline{(u_1' u_1')}_P \tilde{c}(1 - \tilde{c}) + O(1/Da) \end{aligned} \quad (10)$$

The first term on the right-hand side represents the reacting contribution to $\overline{\rho u_1'' u_1'' c''}$, whereas the combined action of second and third terms represent the effects of turbulence on $\overline{\rho u_1'' u_1'' c''}$. The last term $O(1/Da)$ originates from the interior of the flame, and this contribution becomes negligible for $Da \gg 1$. It has been demonstrated elsewhere [44] that the probability density function of c cannot be approximated by a bimodal distribution in the near-wall region. The departure from a bimodal distribution is often quantified in terms of a segregation factor $g = \overline{\rho c''^2} / \bar{\rho} \tilde{c}(1 - \tilde{c})$. Chakraborty and Cant [17,20] utilised the TDH model for the turbulent contribution part in eq. 10 and utilised the segregation factor to propose a model (referred to as the CC model here) for both $Da \gg 1$ and $Da < 1$ combustion based on *a-priori* DNS analyses for the flames without any influence of walls in the following manner:

$$\overline{\rho u_1'' u_1'' c''} = -C_{CS} \frac{\tilde{k}}{\tilde{\varepsilon}} \overline{\rho u_1'' u_1''} \frac{\partial(\overline{\rho u_1'' c''} / \bar{\rho})}{\partial x_1} + \bar{\rho} \left[\frac{\overline{\rho u_1'' c''}}{\bar{\rho} \tilde{c}(1 - \tilde{c})} + \alpha_3 \sqrt{\overline{\rho u_1'' u_1''} / \bar{\rho}} \right]^2 \tilde{c}(1 - \tilde{c})(1 - 2\sqrt{g}\tilde{c})$$

(11)

where $\left[\overline{\rho u_1'' c''} / \{ \bar{\rho} \tilde{c} (1 - \tilde{c}) \} + \alpha_3 \sqrt{\overline{\rho u_1'' u_1''} / \bar{\rho}} \right]$ represents $[(\overline{u_j})_p - (\overline{u_j})_R]$ in eq. 11 where $\alpha_3 = 0.2 + 0.3 \text{erf}(Re_L/20)$ is a model parameter with $Re_L = \rho_0 \tilde{k}^2 / \mu_0 \tilde{c}$ is the local turbulent Reynolds number. The predictions of the CC model (eq. 11) are also shown in Fig. 7, which indicates that the CC model is more successful in capturing the behaviour of $\overline{\rho u_1'' u_1'' c''}$ than the TDH model when the flame is away from the wall, where the CC model reasonably captures both the quantitative and qualitative behaviours of $\overline{\rho u_1'' u_1'' c''}$. However, during flame quenching $\tilde{c}$ approaches 1.0 and as a result the second term on the right-hand side of eq. 11 disappears, and thus the CC model prediction approaches to that of the TDH model in the near-wall region. Thus, the CC model does not adequately capture the near-wall behaviour of $\overline{\rho u_1'' u_1'' c''}$. Here the CC model has been modified in the following manner:

$$\overline{\rho u_1'' u_1'' c''} = -C_{cs} \left(\frac{\tilde{k}}{\tilde{c}} \right) \overline{\rho u_1'' u_1''} \frac{\partial (\overline{\rho u_1'' c''} / \bar{\rho})}{\partial x_1} + \bar{\rho} \tilde{c} (1 - \tilde{c}) (1 - 2g^{0.5(1-\tilde{c}_w)} \tilde{c}) \left[A_w \left(\frac{\overline{\rho u_1'' c''}}{\bar{\rho} \tilde{c} (1 - \tilde{c})} + \alpha_{3w} \sqrt{\frac{\overline{\rho u_1'' u_1''}}{\bar{\rho}}} \right) \right]^2 \quad (12i)$$

where

$$\alpha_{3w} = 0.2[3(1 - \tilde{c}_w)]^{\eta_1} + 0.3 \text{erf}(Re_L/20); \eta_1 = 0.5 \text{erf}[-0.5(x_1/\delta_z - 5(Pe_{min})_L)] \quad (12ii)$$

$$A_w = \exp \left[-\frac{\tilde{c}_w - \tilde{T}_w}{Le} \eta_2 \right]; \eta_2 = 0.5 \text{erf}[-0.5(x_1/\delta_z - (Pe_{min})_L)] \quad (12iii)$$

where $\tilde{c}_w$ and $\tilde{T}_w$ are the Favre averaged value of reaction progress variable and non-dimensional temperature at the wall at a given instant of time. In eq. 12iii $(Pe_{min})_L$ is the minimum Peclet number (where $Pe = X/\delta_z$ is the wall Peclet number with X being the wall normal distance of the $T = 0.9$ isosurface [2,3]) for head-on quenching of laminar premixed flames. For the present thermo-chemistry $(Pe_{min})_L = 3.09, 2.83$ and 2.75 for $Le = 0.8, 1.0$ and 1.2 respectively [44]. These values are consistent with previous experimental [47-49] and

computational [50] analyses. The model parameter α_{3W} is the modified form of α_3 in the CC model, and this modification accounts for the dampening of turbulence close to the wall. The magnitude of $\overline{\rho u_1'' u_1'' c''}$ drops during flame quenching, especially in near-wall region, and the presence of flame close to the wall is sensed by A_w due to an increase in the value of $(\tilde{c}_W - \tilde{T}_W)$ during flame quenching, and this damps the contribution arising from velocity jump across the flame brush due to thermal expansion. The extent of velocity jump across the flame brush is dependent on Le , and thus the damping factor A_w is dependent on Le . Both the TDH and CC models do not adequately predict the negative values of $\overline{\rho u_1'' u_1'' c''}$ close to the wall but this behaviour cannot be captured by $(1 - 2\sqrt{g\tilde{c}})$ because $\overline{\rho c''^2}/\bar{\rho}$ (and thus g) drops drastically during flame quenching. However, the modification $g^{0.5(1-\tilde{c}_W)}$ allows the term $(1 - 2g^{0.5(1-\tilde{c}_W)}\tilde{c})$ to assume negative values during flame quenching when $\tilde{c}_W$ approaches unity (i.e. $\tilde{c}_W \rightarrow 1.0$). It can be seen from Fig. 7 that the model given by eq. 12i (referred to as the new model) predicts both qualitative and quantitative behaviours of $\overline{\rho u_1'' u_1'' c''}$ satisfactorily for both far from and near to the wall for all cases considered here.

It is worth noting that the modifications of model parameters given by eqs. 12ii and 12iii are empirical in nature, but they are proposed in such a manner that the modified model given by eq. 12i asymptotically approaches the previously proposed model for unbounded flows (see eq. 10) away from the wall. The involvements of an exponential function and Re_L in the empirical functions are similar to the van Driest's damping function [24]. Furthermore, the empirical parameters given by eqs. 12ii-iii are taken to be functions of $(Pe_{min})_L$, $\tilde{c}_W$ and $(\tilde{c}_W - \tilde{T}_W)$. The involvement of $(Pe_{min})_L$ implicitly includes the information regarding the flame quenching distance into the model, whereas the $(\tilde{c}_W - \tilde{T}_W)$ dependence of the model parameter ensures that the effects of enthalpy loss due to wall heat transfer are reflected in the qualitative and

quantitative variations of $\overline{\rho u_1'' u_1'' c''}$ depending on the distance of the flame from the wall (see Fig. 2 to observe that the value of $\tilde{c}_W$ changes with time). As the value of $\tilde{c}_W$ changes with time (it remains 0 when the flame is away from the wall, but it increases from 0 and approaches 1.0 with the advancement of quenching), the dependence of $\tilde{c}_W$ in the model parameters acts as the sensor of flame position from the wall. Similar modelling approaches were previously adopted by Bruneaux *et al.* [51] and Alshaalan *et al.* [52] in the context of FSD closures for wall-bound turbulent premixed flames.

4.5 Modelling of the pressure gradient terms ($T_4 + T_5$)

Both the mean and fluctuating pressure terms are often modelled in a combined manner due to their similar origin [17,20,24]. There are several available models for the closure of $(T_4 + T_5)$. Three of these models take the following form by combining conventional closures of slow and rapid terms [24]:

$$T_4 + T_5 = -C_{1c} \frac{\tilde{\epsilon}}{\tilde{k}} \overline{\rho u_i'' c''} + C_{2c} \overline{\rho u_k'' c''} \frac{\partial \tilde{u}_i}{\partial x_k} + C_{3c} \overline{\rho u_k'' c''} \frac{\partial \tilde{u}_k}{\partial x_i} + C_{4c} \overline{\rho u_i'' u_k''} \frac{\partial \tilde{c}}{\partial x_k} \quad (13)$$

where the slow part is represented by $-C_{1c}(\tilde{\epsilon}/\tilde{k})\overline{\rho u_i'' c''}$ and the rapid part is given by: $C_{2c}\overline{\rho u_k'' c''}(\partial \tilde{u}_i/\partial x_k) + C_{3c}\overline{\rho u_k'' c''}(\partial \tilde{u}_k/\partial x_i) + C_{4c}\overline{\rho u_i'' u_k''}(\partial \tilde{c}/\partial x_k)$ with C_{1c} , C_{2c} , C_{3c} and C_{4c} being the model parameters. Launder [53] suggested that $C_{1c} = 3.0$, $C_{2c} = 0$, $C_{3c} = 0$ and $C_{4c} = 0.4$, and this model will henceforth be referred to the PL model. Craft [54] adopted a similar model (referred to as the PC model) with $C_{1c} = 3.0$, $C_{2c} = 0.5$, $C_{3c} = 0$ and $C_{4c} = 0$. Durbin [55] suggested an alternative model (PD model) where $C_{1c} = 2.5$, $C_{2c} = 0$, $C_{3c} = 0$ and $C_{4c} = 0.45$. In addition, Jones [56] and Bradley *et al.* [57] proposed alternative models for $(T_4 + T_5)$ in the following manner:

$$T_4 + T_5 = -\overline{c''} \frac{\partial \bar{P}}{\partial x_i} - C_{\phi 1} \frac{\tilde{\epsilon}}{\tilde{k}} \overline{\rho u_i'' c''} + C_{\phi 2} \overline{\rho u_k'' c''} \frac{\partial \tilde{u}_i}{\partial x_k} \quad (14)$$

Jones [56] considered $C_{\phi_1} = 3.0$ and $C_{\phi_2} = 0.5$ for this (PJ model) model. By contrast, Bradley *et al.* [57] chose $C_{\phi_1} = 3.0$ and $C_{\phi_2} = 0$ for their model (PB model). Another alternative model (PLV model) was proposed by Lindstedt and Vaos [32]:

$$T_4 + T_5 = -\overline{c''} \frac{\partial \bar{P}}{\partial x_i} + \overline{\rho u_i'' c''} G_{il} + C_{As} \overline{c''} \frac{\partial \bar{P}}{\partial x_i} \quad (15)$$

where $C_{As} = 1/3$ and G_{il} is the generalized Langevin coefficient which is a function of Reynolds stress $\overline{\rho u_i'' u_j''}$ and the mean velocity gradient $\partial \tilde{u}_l / \partial x_j$ [32]. Domingo and Bray [58] proposed a model expression (PDB model) for the strict flamelet burning of premixed turbulent flames:

$$T_4 + T_5 = \frac{\tilde{c}(1-\tilde{c})}{(1+\tau\tilde{c})} \left[-\frac{\partial \bar{P}_R}{\partial x_i} + (1+\tau) \frac{\partial \bar{P}_P}{\partial x_i} \right] - 0.5(\vec{N} \cdot \vec{M}_l) \tau \cdot \rho_0 S_L^2 (0.7 - \tilde{c}) \Sigma_{\text{gen}} \quad (16)$$

where $\bar{P}_R$ and $\bar{P}_P$ represent the conditional mean pressure in reactants and products respectively, $\vec{N} = -\nabla c / |\nabla c|$ is the local flame normal vector and $\vec{M}_l$ is the unit vector in the x_i -direction. Nishiki *et al.* [13] proposed the following model (PN model) based on *a-priori* DNS analysis:

$$T_4 + T_5 = -C_D \frac{\bar{p}}{\rho_0} \cdot \tilde{c}(1-\tilde{c}) \tau \frac{\partial \bar{P}}{\partial x_i} - C_{E1} \frac{\tilde{\varepsilon}}{\bar{k}} \overline{\rho u_i'' c''} + C_{E2} \tau \cdot S_L \bar{W} (1-\tilde{c})^{1.7} \quad (17)$$

where $C_D = 0.8$, $C_{E1} = 0.38$ and $C_{E2} = 0.66$ model constants. In the context of BML analysis $\overline{c''}$ can be expressed as $\overline{c''} = (\bar{\rho}/\rho_0) \tilde{c}(1-\tilde{c}) \tau$ when the pdf of c can be assumed to follow a bimodal distribution with impulses at $c = 0$ and $c = 1.0$ [2]. Thus, the first term on the right hand side of eq. 17 accounts for the contribution of $T_4 = -\overline{c''} \partial \bar{P} / \partial x_i$.

The predictions of all these model are compared to $(T_4 + T_5)$ extracted from DNS data for cases A, C and E in Fig. 8 for different time instants. It is clear from Fig. 8 that each of the PL, PC and PD models exhibit negative values for all cases, and fail to capture both the qualitative

and quantitative behaviours of $(T_4 + T_5)$ extracted from DNS data. These models (i.e. PL, PC and PD models) were originally proposed for incompressible non-reacting flows [53-55] where the contribution of $-\overline{c''} \partial \overline{P} / \partial x_i$ was ignored. However, it can be seen from Fig. 6 that T_4 plays a key role in turbulent scalar flux transport in turbulent premixed flames so it is not surprising that the PL, PC and PD models do not adequately capture the behaviour of $(T_4 + T_5)$. The PJ model predicts positive values of $(T_4 + T_5)$ but overpredicts the magnitude obtained from DNS data in case A. The quantitative agreement between the PJ model and DNS data in case C is better than case A. However, the prediction of the PJ model does not adequately capture the behaviour of $(T_4 + T_5)$ for high values of $u'/S_L \sim Re_t^{1/4} Ka^{1/2} \sim Re_t^{1/2} Da^{-1/2}$ (e.g. case E) and at some time instants (e.g. $t \geq 6 \delta_Z/S_L$) this model also does not even predict the correct qualitative behaviour. The PB model satisfactorily captures the qualitative behaviour of $(T_4 + T_5)$ with some underprediction for case A until $t \leq 8 \delta_Z/S_L$. However, the PB model locally overpredicts $(T_4 + T_5)$ at the later times (see $t > 10 \delta_Z/S_L$). The PB model shows some qualitative agreement with DNS data in cases C and E at early times when the flame is away from the wall (e.g. $t = 4 \delta_Z/S_L$), whereas both the qualitative and quantitative agreement remain poor at later times when the flame quenching is in progress.

The PLV model captures the qualitative behaviour of DNS in case A, but it overpredicts the magnitude of $(T_4 + T_5)$ for all time steps. For cases with high $u'/S_L \sim Re_t^{\frac{1}{4}} Ka^{\frac{1}{2}} \sim Re_t^{\frac{1}{2}} Da^{-\frac{1}{2}}$ (e.g. cases C and E) the PLV model overpredicts the DNS data for $t \leq 6 \delta_Z/S_L$ when the flame is away from the wall. As the flame approaches the wall the PLV models fails to capture both quantitative and qualitative behaviours obtained from DNS data. Whilst the PDB model captures the qualitative behaviour but overpredicts the magnitude of $(T_4 + T_5)$ for case A when the flame is away from the wall (e.g. $t = 4 \delta_Z/S_L$). As the flame starts to approach the wall the

PDB model predicts negative values whereas $(T_4 + T_5)$ remains positive. The predictions of the PDB model do not perform satisfactorily for high $u'/S_L \sim Re_t^{1/4} Ka^{1/2} \sim Re_t^{1/2} Da^{-1/2}$ cases (e.g. cases C and E) and the predictions show large extent of noise. This noise originates due to limited sample size in the evaluation of conditional mean pressures $\bar{P}_R$ and $\bar{P}_P$. This spiky behaviour was also reported in the original paper by Domingo and Bray [58] and previous analyses [17,20] which dealt with this model. The PDB model was originally proposed for the strict flamelet regime (i.e. $Ka < 1$ and $Da > 1$) where the pdf of c can be approximated by a bimodal distribution with impulses at $c = 0$ and 1.0 but such an assumption is not valid for the flames (where $Ka > 1$ and $Da < 1$) considered here. Furthermore, it has been shown earlier [44] that the pdf of c does not show bimodality at any stage of head-on quenching, so it is not surprising that the PDB model does not adequately capture the behaviour of $(T_4 + T_5)$ during flame quenching.

Finally, the PN model captures both the qualitative and quantitative behaviours of $(T_4 + T_5)$ better than the other alternative models. However, for high values of $u'/S_L \sim Re_t^{1/4} Ka^{1/2} \sim Re_t^{1/2} Da^{-1/2}$ the PN model overpredicts the behaviour of $(T_4 + T_5)$. The agreement with the PN model prediction and $(T_4 + T_5)$ from DNS data deteriorates at later times during flame quenching for all cases.

The models (e.g. PL, PC, PD models) which neglected the leading contribution of $T_4 = -\overline{c''} \partial \bar{P} / \partial x_i$ are not successful in capturing the DNS data. However, the PJ, PB and PN models, which account for $T_4 = -\overline{c''} \partial \bar{P} / \partial x_i$ are more successful in capturing the behaviour of $(T_4 + T_5)$ than the PL, PC, PD models which ignore this contribution. However, some near-

wall corrections are needed to account for the behaviour of $(T_4 + T_5)$ during flame quenching.

Here the following near-wall modification has been suggested for the PN model:

$$T_4 + T_5 = -C_D \frac{\bar{\rho}}{\rho_0} \tilde{c}(1 - \tilde{c})\tau \frac{\partial \bar{P}}{\partial x_i} - C_{E1}^* \frac{\tilde{\epsilon}}{\tilde{k}} \overline{\rho u_i'' c''} + C_{E2}^* \tau \cdot S_L [\rho_0 S_L \Sigma_{gen}] (1 - \tilde{c})^{1.7} \quad (18)$$

where $C_{E1}^* = 0.38\eta_3 5^{1-0.5[\text{erf}(x_1/\delta_Z - \Psi)+1]}$, $C_{E2}^* = 0.66\eta_3^{1-0.5[\text{erf}(5(\tilde{c}_W - 0.5))+1]}$ and $\eta_3 = 0.5[\text{erf}(x_1/\delta_Z - 0.5(Pe_{min})_L) + 1]$ are the model parameters and $\Psi = 0.5(Pe_{min})_L(\text{erf}(8Le - 6) + 1)$ is the parameterisation of minimum Peclet number for turbulent flames as proposed earlier by Lai and Chakraborty [44]. This parameterisation accounts for the finding by Lai and Chakraborty [44] that the minimum wall Peclet number Pe_{min} for turbulent flames remains comparable to the corresponding laminar flame value $(Pe_{min})_L$ for $Le = 1.0$ and 1.2 cases, but for $Le=0.8$ cases, Pe_{min} assumes a smaller magnitude than the corresponding $(Pe_{min})_L$. Interested readers are referred to Ref. [44] for further discussion on wall Peclet number behaviour in head-on quenching of turbulent premixed flames. The involvement of error functions in the model parameters C_{E1}^* and C_{E2}^* ensure that they approach asymptotically to $C_{E1} = 0.38$ and $C_{E2} = 0.66$ away from the wall in the absence of flame quenching. The involvement of $\Sigma_{gen} = |\overline{\nabla c}|$ in the third term on the right-hand side of eq. 18 allows for a non-zero prediction at the wall which is identically zero in the PN model because $\bar{w}$ vanishes at the wall due to flame quenching. The involvement of $(Pe_{min})_L$ and Ψ in C_{E1}^* and η_3 implicitly includes the information regarding the flame quenching distance into the revised model, whereas $\tilde{c}_W$ dependence of C_{E2}^* senses the flame quenching and modifies the value accordingly. It can be seen from Fig. 8 that the modified PN model (eq. 18) captures the near-wall behaviour of $(T_4 + T_5)$ during flame quenching better than any other available models.

4.6 Modelling of the molecular dissipation terms $(T_6 + T_7)$

The terms T_6 and T_7 tend to reduce the magnitude of the scalar flux (i.e. behaves as a sink), and are usually modelled together. The most common model for $(T_6 + T_7)$ is the one which was proposed in the context of BML analysis [2] (i.e. referred to as the DBML model in this analysis):

$$T_6 + T_7 = -K_1 \overline{\rho u_i'' c''} \frac{\bar{w}}{[\bar{\rho} \tilde{c}(1-\tilde{c})]} \quad (19)$$

where $K_1 \approx 0.85$ is the model parameter. An alternative model was proposed by Nishiki *et al.* [13] (DN model) in the following manner:

$$T_6 + T_7 = -C_F \tau S_L \bar{w} \quad (20)$$

where $C_F \approx 0.4$ is the model parameter. However, eq. 20 is only valid for counter-gradient transport, and thus Chakraborty and Cant [20] suggested a combination of DBML and DL model, which was shown previously to model $(T_6 + T_7)$ satisfactorily even for low Damköhler number combustion without the influence of walls. The expression proposed by Chakraborty and Cant [17,20] (DC model) is given by:

$$T_6 + T_7 = -0.5 C_F \tau S_L \bar{w} - 0.5 K_1 \overline{\rho u_i'' c''} \times \frac{\bar{w}}{[\bar{\rho} \tilde{c}(1-\tilde{c})]} \quad (21)$$

The predictions of the DBML, DN and DC models are compared to $(T_6 + T_7)$ extracted from DNS data in Fig. 9. It can be seen from Fig. 9 that the DBML model captures the correct qualitative behaviour of $(T_6 + T_7)$ but it underestimates the negative contribution of $(T_6 + T_7)$ in cases C-E. For cases A and B, the DBML model underpredicts both negative (away from the wall) and positive (when the flame is close to the wall) contribution of $(T_6 + T_7)$. The DN model provides a satisfactory qualitative prediction of $(T_6 + T_7)$ for all cases but this model overpredicts the magnitude of negative contribution of $(T_6 + T_7)$ for $t \geq 6 \delta_Z/S_L$ in cases A and B. In other cases the DN model exhibits overprediction of the magnitude of the negative contribution of $(T_6 + T_7)$. The agreement between the DC model prediction and DNS data

remains better than the DBML and DN models. However, the DC model still underpredicts (overpredicts) the magnitude of positive (negative) contribution of $(T_6 + T_7)$ for all cases considered here but the extent of overprediction of the negative value is much smaller in extent in comparison to the DN model. It can further be seen from Fig. 9 that all the available models (i.e. DBML, DN and DC models) cannot predict the non-zero contributions of $(T_6 + T_7)$ in the near-wall region (and at the wall) because T_7 exhibits non-zero values even when the flame is quenched (i.e. $\bar{w} = 0$). To avoid this problem, the following modification to the DN model is proposed here (referred to here as the new model):

$$(T_6 + T_7) = -0.5C_F\tau S_L(\rho_0 S_L \Sigma_{\text{gen}} Q^p) - 0.5K_1 \overline{\rho u_i'' c''} \times \frac{\bar{w}}{[\bar{\rho} \tilde{c}(1-\tilde{c})]} \quad (22i)$$

$$\text{where } Q = \text{erf}[2(\tilde{c}_W - 0.5)] \text{ and } p = 0.5[\text{erf}(x_1/\delta_Z - 0.7(Pe_{\min})_L) + 1] \quad (22ii)$$

The involvement of $\Sigma_{\text{gen}} = |\nabla c|$ allows for a non-zero prediction at the wall which was not possible by the other alternative models. At the beginning of quenching, a positive value of $(T_6 + T_7)$ is obtained at the wall, but it becomes negative at later stages. The model parameter Q accounts for the change of sign of $(T_6 + T_7)$ depending on the value of Favre averaged progress variable at the wall $\tilde{c}_W$, whereas p ensures that Q^p modifies the magnitude of eq. 22i to predict $(T_6 + T_7)$ extracted from DNS data. Here, $(Pe_{\min})_L$ dependence of p implicitly accounts for the information regarding the flame quenching distance, and the error functions in eq. 22ii ensure that eq. 22i approaches eq. 21 for $x_1/\delta_Z \gg (Pe_{\min})_L$. It is evident from Fig. 9 that the model given by eq. 24i satisfactorily captures both qualitative and quantitative behaviours of $(T_6 + T_7)$ both away from and close to the wall.

4.7 Modelling of the reaction rate velocity correlation term T_8

The model proposed for the reaction rate velocity correlation term $T_8 = \overline{u_i'' \dot{w}}$ in the context of BML analysis (referred to as the RB model here) takes the form [2]:

$$T_8 = C_R(\varphi_m - \tilde{c}) \overline{\dot{w}} \frac{\overline{\rho u_i'' c''}}{\rho c''^2} \quad (23)$$

where the model parameters are given by $C_R \approx 1$ and $\varphi_m \approx 0.5$. *A-priori* DNS analysis by Chakraborty and Cant [20] showed that the RB model captures the qualitative behaviour of T_8 even for low Damköhler number (i.e. $Da < 1$) combustion but revealed some turbulent Reynolds number dependence of φ_m and the following parameterisation was proposed for φ_m :

$$\varphi_m = 0.57 + 0.6 \operatorname{erfc}[(Re_L + 1)/10] \quad (24)$$

Equation 23 with φ_m parameterisation given by eq. 24 will henceforth be referred to as the RB-M model. The predictions of the RB and RB-M models are compared to T_8 extracted from DNS data in Fig. 10 for cases A, C and E for different time instants. Figure 10 shows that the RB model captures quantitative and qualitative behaviours of T_8 for case A before the initiation of flame quenching (i.e. $t \leq 6 \delta_Z/S_L$). However, this model overpredicts the magnitude of positive and negative values of T_8 close to the wall and away from the wall respectively for case A at $t > 6 \delta_Z/S_L$. For cases C-E, the RB model overpredicts of both negative (away from wall region) and positive (near-wall region) values of T_8 . As the flame propagates towards the wall and the flame starts to quench, the RB model fails to predict the reaction rate velocity correlation term T_8 , as shown in Fig. 10. By contrast, the RB-M model captures both quantitative and qualitative behaviour of reaction rate-velocity correlation term T_8 more satisfactorily than the RB model in spite of slight underprediction of T_8 for cases with high values of $u'/S_L \sim Re_t^{\frac{1}{4}} Ka^{\frac{1}{2}} \sim Re_t^{\frac{1}{2}} Da^{-\frac{1}{2}}$ (e.g. cases D and E). The prediction of T_8 can further be improved by modifying the RB-M model in the following manner (i.e. new model):

$$T_8 = C_R(\varphi_m \exp[2(\tilde{c}_W - \tilde{T}_W)\xi] - \tilde{c})\bar{w} \times \frac{\overline{\rho u_i'' c''}}{\rho c''^2} \text{ where } \xi = 1 - 0.5[\text{erf}(x_1/\delta_Z - (Pe_{min})_L) + 1] \quad (25)$$

The factor $(\varphi_m \exp[2(\tilde{c}_W - \tilde{T}_W)\xi] - \tilde{c})$ approaches $(\varphi_m - \tilde{c})$ for $x_1/\delta_Z \gg (Pe_{min})_L$. A comparison between the predictions of the RB-M and the new model indicates that $(\varphi_m \exp[2(\tilde{c}_W - \tilde{T}_W)\xi] - \tilde{c})$ in eq. 25 modifies the RB-M model close to the wall depending on the value of $(\tilde{c}_W - \tilde{T}_W)$ to yield better agreement with model prediction with T_8 extracted from DNS data than the other available models especially in the vicinity of the wall.

The modifications to the models proposed here and the reference models which were modified are summarised in Table 3 for the convenience of the readers and future users. The modified models approach the reference models for $x_1/\delta_Z \gg (Pe_{min})_L$. The combined contribution of $(T_1 + T_2 + T_3 + T_4 + T_5 + T_6 + T_7 + T_8)$ as obtained from DNS data is compared to the corresponding term according to the combined predictions of eqs. 12i, 18, 22i and 25 in Fig. 11 and it can be seen the modified models capture the behaviour of $(T_1 + T_2 + T_3 + T_4 + T_5 + T_6 + T_7 + T_8)$ in a better manner than the models without wall corrections in most locations within the flame brush for all Lewis number and turbulent intensities considered here but disagreements between the local behaviours of these quantities have been observed in some cases (e.g. case E with $Le = 0.8$ shows this disagreement due to inaccuracy in the modelling of $(T_4 + T_5)$ at $t = 2\delta_Z/S_L$).

5. CONCLUSIONS

The modelling of turbulent scalar flux $\overline{\rho u_i'' c''}$ transport has been analysed for head-on quenching of statistically planar turbulent premixed flames by an isothermal wall using three-dimensional DNS data for different values of Damköhler and Karlovitz numbers for global

Lewis number $Le = 0.8 - 1.2$. The statistical behaviour of the unclosed terms of the transport equation of $\overline{\rho u_i'' c''}$, especially in the near-wall region, has been analysed in detail. The magnitudes of the turbulent transport and mean velocity gradient terms remain small in comparison to the contributions of the other terms when the flame is away from the wall but the magnitudes of all the terms diminish during flame-wall interaction and become comparable at the final stage of quenching before vanishing altogether. The effects of turbulence become weak at advanced stages of head-on quenching and this is particularly prominent in the near-wall region for this configuration. Thus, in this configuration it is necessary for the closures of scalar flux transport to perform well in relatively strong turbulent regions within the flame but also in the weakly turbulent near-wall zones at advanced stages of flame quenching. The modelling of the unclosed terms has been addressed in detail and it has been found that existing models for the turbulent transport, pressure gradient, molecular dissipation and velocity-reaction rate terms do not adequately capture the behaviour of these terms close to the wall. The models for the turbulent transport, pressure gradient, molecular dissipation and velocity-reaction rate terms have been modified in terms of blending functions, similar to the van Driest's correction for mixing length used for damping eddy viscosity close to the wall [24] in such a manner that the models satisfactorily capture the behaviour obtained from DNS data both close to the wall and far from it. Furthermore, the model modifications are considered to be functions of the non-dimensional quenching distance (i.e. minimum Peclet number) and the quenching sensors in the form of $\tilde{c}_w$ and $(\tilde{c}_w - \tilde{T}_w)$.

The statistical behaviour of scalar flux and its transport is dependent on the competition between the rms turbulent velocity fluctuation u' and the typical velocity jump across the flame brush, quantified τS_L [5,6,8,16-18], and this competition is quantified in terms of Bray number N_B [5,16-18]. Thus, the physical mechanisms responsible for gradient or counter gradient

transport will not be different even if one uses a complex chemical mechanism instead of a single step chemical reaction. This has been confirmed by a recent analysis by Klein *et al.* [59], which indicated that the statistical behaviours of sub-grid scalar flux behaviour obtained from a detailed chemistry DNS database for nominally thermo-diffusively neutral H₂-air flames remain qualitatively similar to the behaviours observed from simple chemistry DNS databases [21-22]. Moreover, several previous analyses [5-23] on turbulent scalar flux employed simple chemistry to gain fundamental physical insights and the same approach has been adopted here. However, further validation based on three-dimensional DNS and experimental data with detailed thermochemistry will be necessary for more comprehensive validation of the models discussed here. Several analyses [5-23] in the past concentrated only on *a-priori* analysis and the same approach has been adopted here. However, the models proposed here have to be implemented in actual RANS simulations for configurations with well-documented experimental data for the purpose of *a-posteriori* assessment, which is kept beyond the scope of this analysis. In actual RANS simulations, the numerical errors and modelling inaccuracies interact with each other and thus it is not straightforward to extract modelling inaccuracies from the simulation results. Besides, any *a-posteriori* analysis is also expected to be code-dependent. Furthermore, in turbulent combustion simulations, the quantities related to fluid turbulence (e.g. $\tilde{k}$ and $\tilde{\epsilon}$) act as input parameters to the scalar flux and combustion models and thus turbulence, scalar flux and combustion models interact in a complex manner in actual RANS simulations. As species field affects the velocity distribution in reacting flows, even two sets of RANS simulations with the new turbulent scalar flux transport models and without them, will not be able to isolate whether the differences in the simulation results arise only due to turbulent scalar flux closures or due to a coupling of species and velocity fields. Further analysis of the closures for turbulent scalar flux $\overline{\rho u_i'' c''}$ transport based on detailed chemistry DNS data along with *a-posteriori* validation will form the basis of future investigations.

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TABLES

Case	A	B	C	D	E
u'/S_L	5.0	6.25	7.5	9.0	11.25
L_{11}/δ_{th}	1.67	1.44	2.5	4.31	3.75
Da	0.33	0.23	0.33	0.48	0.33
Ka	8.65	13.0	13.0	13.0	19.5
Re_t	22.0	23.5	49.0	100	110

Table 1: List of initial simulation parameters away from the wall for each of the Lewis number cases.

		Case A		Case B		Case C		Case D		Case E	
	tS_L/δ_z	A_T/A_L	S_T/S_L	A_T/A_L	S_T/S_L	A_T/A_L	S_T/S_L	A_T/A_L	S_T/S_L	A_T/A_L	S_T/S_L
$Le = 0.8$	1	1.62	1.61	1.69	1.68	3.50	3.47	3.26	3.23	5.33	5.29
	2	2.49	2.48	2.63	2.63	4.05	4.05	5.74	5.73	6.71	6.70
	4	2.64	2.62	2.36	2.35	2.69	2.67	2.32	2.30	1.50	1.48
	6	1.90	1.88	1.70	1.68	0.44	0.43	0.28	0.28	0.15	0.15
	8	0.94	0.93	1.07	1.06	0.04	0.04	0.03	0.03	0.02	0.02
	10	0.17	0.17	0.19	0.19	0.01	0.01	0.01	0.01	0.01	0.01
$Le = 1.0$	1	1.57	1.55	1.59	1.57	2.79	2.78	2.91	2.90	4.18	4.17
	2	1.67	1.66	1.60	1.59	2.99	2.99	3.95	3.93	4.77	4.76
	4	1.77	1.76	1.73	1.71	2.34	2.31	2.39	2.37	2.03	2.01
	6	1.64	1.62	1.68	1.66	1.43	1.41	0.74	0.74	0.68	0.67
	8	1.51	1.49	1.53	1.51	0.50	0.49	0.20	0.19	0.12	0.12
	10	0.86	0.85	0.85	0.84	0.09	0.09	0.03	0.03	0.03	0.03
$Le = 1.2$	1	1.29	1.28	1.22	1.21	1.92	1.91	2.04	2.02	2.68	2.66
	2	1.38	1.37	1.33	1.32	2.01	2.00	2.75	2.74	3.43	3.43
	4	1.31	1.30	1.28	1.27	1.82	1.81	1.98	1.96	1.57	1.55
	6	1.30	1.29	1.29	1.28	1.60	1.59	1.51	1.49	1.23	1.22
	8	1.23	1.22	1.24	1.23	1.12	1.11	0.60	0.60	0.47	0.46
	10	1.15	1.14	1.14	1.13	0.60	0.60	0.18	0.18	0.10	0.10

Table 2: List of normalised flame surface area A_T/A_L and turbulent flame speed S_T/S_L at different stages of flame quenching for all cases considered here.

Term	Reference model	Modified model
$\overline{\rho u_1'' u_1'' c''}$	$-C_{CS} \frac{\tilde{k}}{\tilde{\varepsilon}} \overline{\rho u_1'' u_1''} \frac{\partial(\overline{\rho u_1'' c''}/\bar{\rho})}{\partial x_1} +$ $\bar{\rho} \left[\frac{\overline{\rho u_1'' c''}}{\bar{\rho} \tilde{c}(1-\tilde{c})} + \right.$ $\left. \alpha_3 \sqrt{\overline{\rho u_1'' u_1''}/\bar{\rho}} \right]^2 \tilde{c}(1-\tilde{c})(1 - 2\sqrt{g\tilde{c}})$ $C_{CS} = 0.22$ $\alpha_3 = 0.2 + 0.3\text{erf}(Re_L/20)$	$-C_{CS} \left(\frac{\tilde{k}}{\tilde{\varepsilon}} \right) \overline{\rho u_1'' u_1''} \frac{\partial(\overline{\rho u_1'' c''}/\bar{\rho})}{\partial x_1}$ $+ \bar{\rho} \tilde{c}(1-\tilde{c}) \left(1 - 2g^{0.5(1-\tilde{c}_W)} \tilde{c} \right) \left[A_w \left(\frac{\overline{\rho u_1'' c''}}{\bar{\rho} \tilde{c}(1-\tilde{c})} \right) \right.$ $\left. + \alpha_{3W} \sqrt{\frac{\overline{\rho u_1'' u_1''}}{\bar{\rho}}} \right]^2$ $\alpha_{3W} = 0.2[3(1-\tilde{c}_W)]^{\eta_1} + 0.3\text{erf}(Re_L/2)$ $\eta_1 = 0.5\text{erf}[-0.5(x_1/\delta_Z - 5(Pe_{min})_L)]$ $A_w = \exp \left[-\frac{\tilde{c}_W - \tilde{T}_W}{Le} \eta_2 \right]$ $\eta_2 = 0.5\text{erf}[-0.5(x_1/\delta_Z - (Pe_{min})_L)]$
$T_4 + T_5$	$-C_D \frac{\bar{\rho}}{\rho_0} \cdot \tilde{c}(1-\tilde{c}) \tau \frac{\partial \bar{P}}{\partial x_i}$ $- C_{E1} \frac{\tilde{\varepsilon}}{\tilde{k}} \overline{\rho u_i'' c''}$ $+ C_{E2} \tau \cdot S_L \bar{W} (1 - \tilde{c})^{1.7}$ $C_D = 0.8$ $C_{E1} = 0.38$ $C_{E2} = 0.66$	$-C_D \frac{\bar{\rho}}{\rho_0} \cdot \tilde{c}(1-\tilde{c}) \tau \frac{\partial \bar{P}}{\partial x_i} - C_{E1}^* \frac{\tilde{\varepsilon}}{\tilde{k}} \overline{\rho u_i'' c''} +$ $C_{E2}^* \tau \cdot S_L [\rho_0 S_L \Sigma_{gen}] (1-\tilde{c})^{1.7}$ $C_D = 0.8$ $C_{E1}^* = 0.38 \eta_3 5^{1-0.5[\text{erf}(x_1/\delta_Z - \Psi) + 1]}$ $C_{E2}^* = 0.66 \eta_3^{1-0.5[\text{erf}(5(\tilde{c}_W - 0.5)) + 1]}$ $\eta_3 = 0.5[\text{erf}(x_1/\delta_Z - 0.5(Pe_{min})_L) + 1]$ $\Psi = 0.5(Pe_{min})_L (\text{erf}(8Le - 6) + 1)$
$T_6 + T_7$	$-0.5 C_F \tau S_L \bar{W} - 0.5 K_1 \overline{\rho u_i'' c''}$ $\times \frac{\bar{W}}{[\bar{\rho} \tilde{c}(1-\tilde{c})]}$ $C_F = 0.4$	$-0.5 C_F \tau S_L (\rho_0 S_L \Sigma_{gen} Q^p) - 0.5 K_1 \overline{\rho u_i'' c''}$ $\times \frac{\bar{W}}{[\bar{\rho} \tilde{c}(1-\tilde{c})]}$ $Q = \text{erf}[2(\tilde{c}_W - 0.5)]$ $p = 0.5[\text{erf}(x_1/\delta_Z - 0.7(Pe_{min})_L) + 1]$
T_8	$C_R (\varphi_m - \tilde{c}) \bar{W} \frac{\overline{\rho u_i'' c''}}{\rho c''^2}$ $C_R = 1$ $\varphi_m = 0.57 + 0.6\text{erfc}[(Re_L + 1)/10]$	$C_R (\varphi_m \exp[2(\tilde{c}_W - \tilde{T}_W)\xi] - \tilde{c}) \bar{W} \times \frac{\overline{\rho u_i'' c''}}{\rho c''^2}$ $\xi = 1 - 0.5[\text{erf}(x_1/\delta_Z - (Pe_{min})_L) + 1]$

Table 3: Summary of the modified models proposed here along with the reference models which were modified.

FIGURE CAPTIONS

Figure 1: (a) Schematic diagram of head-on quenching of a statistically planar flame, (b) schematic diagram of the computational domain, (c) Instantaneous $\mathbf{c}$ and $\mathbf{T}$ fields for cases A, C and E (1st -3rd column) at $t = 2 \delta_z/S_L, 4 \delta_z/S_L$ and $6 \delta_z/S_L$ (1st -3rd row).

Figure 2: (a) Variation of $\tilde{c}$ with x_1/δ_z (log scale) for cases A, C and E (1st -3rd column) at $t = 2 \delta_z/S_L, 6 \delta_z/S_L$ and $10 \delta_z/S_L$ (1st -3rd row). (b) Temporal evolution of the maximum, mean and minimum values of non-dimensional wall heat flux Φ_w for cases A, C and E (1st -3rd column). Vertical black broken lines are indicating $t = 2\delta_z/S_L, 6\delta_z/S_L$ and $8\delta_z/S_L$ (left to right).

Figure 3: Variation of $\overline{\rho u_1'' c''}/(\rho_0 S_L)$ with x_1/δ_z (log scale) for cases A, C and E (1st -3rd column) at $t = 2 \delta_z/S_L, 6 \delta_z/S_L$ and $10 \delta_z/S_L$ (1st -3rd row).

Figure 4: Variation of $\overline{\rho u_1'' c''} \times \partial \tilde{c} / \partial x_1 \times \delta_{th} / (\rho_0 S_L)$ with x_1/δ_z (log scale) for cases A, C and E (1st -3rd column) at $t = 2 \delta_z/S_L, 6 \delta_z/S_L$ and $10 \delta_z/S_L$ (1st -3rd row).

Figure 5: (a) Variations of (a) $\sqrt{2\tilde{k}/3}/S_L$ (—), $\tilde{k}^{3/2}/\tilde{c}/\delta_{th}$ (—) and (b) Ka_L (—) and Da_L (—) with x_1/δ_z (log scale) for cases A, C and E (1st -3rd column) at $t = 2 \delta_z/S_L, 6 \delta_z/S_L$ and $10 \delta_z/S_L$ (1st -3rd row). For illustration purpose $\tilde{c}$ is indicated by background colour.

Figure 6: Variation of the terms $T1$ (—), $T2$ (—), $T3$ (—), $T4$ (—), $T5$ (—), $T6$ (—), $T7$ (—) and $T8$ (—) with x_1/δ_z for cases A, C and E (1st -3rd column) at $t = 2 \delta_z/S_L, 6 \delta_z/S_L$ and $10 \delta_z/S_L$ (1st -3rd row). All the terms are non-dimensionalised by $\rho_0 S_L^2 / \delta_z$.

Figure 7: Variation of $\overline{\rho u_1'' u_1'' c''} / \rho_0 S_L^2$ from DNS data (—), TDH (—), CC (—) and New model (—) with x_1/δ_z (log scale) for cases A, C and E (1st -3rd column) at $t = 2 \delta_z/S_L, 6 \delta_z/S_L$ and $10 \delta_z/S_L$ (1st -3rd row).

Figure 8: Variation of terms $(T_4 + T_5) \times \delta_z / \rho_0 S_L^2$ from DNS data (—), PN (—), PC (—+—), PD (—◇—), PJO (—□—), PLV (—○—), PDB(—▷—), Modified PN model (—) with x_1/δ_z (log scale) for cases A, C and E (1st -3rd column) at $t = 2 \delta_z/S_L, 6 \delta_z/S_L$ and $10 \delta_z/S_L$ (1st -3rd row).

Figure 9: Variation of $(T_6 + T_7) \times \delta_z / \rho_0 S_L^2$ from DNS data (—), DBML (—), DN (—) and CC (—) and New model (—) with x_1/δ_z (log scale) for cases A, C and E (1st -3rd column) at $t = 2 \delta_z/S_L, 6 \delta_z/S_L$ and $10 \delta_z/S_L$ (1st -3rd row).

Figure 10: Variation of $T_8 \times \delta_z / \rho_0 S_L^2$ from DNS data (—), RB (—), RBM (— —) and New model (—) with x_1/δ_z (log scale) for cases A, C and E (1st -3rd column) at $t = 2 \delta_z/S_L, 6 \delta_z/S_L$ and $10 \delta_z/S_L$ (1st -3rd row).

Figure 11: Variation of $(T_1 + T_2 + T_3 + T_4 + T_5 + T_6 + T_7 + T_8) \times \delta_z / \rho_0 S_L^2$ from DNS data (—), and combined model predictions according to eqs. 12i, 18, 22i and 25 (—) and the reference models without wall correction (see Table 3) (—) with x_1/δ_z (log scale) for cases A, C and E (1st -3rd column) at $t = 2 \delta_z/S_L, 6 \delta_z/S_L$ and $10 \delta_z/S_L$ (1st -3rd row).

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Figure 4: Variation of $\overline{\rho u_1'' c''} \times \frac{\partial \tilde{c}}{\partial x_1} \times \delta_{th} / (\rho_0 S_L)$ with x_1 / δ_Z (log scale) for cases A, C and E (1st -3rd column) at $t = 2 \delta_Z / S_L$, $6 \delta_Z / S_L$ and $10 \delta_Z / S_L$ (1st -3rd row).

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Figure 7: Variation of terms $\overline{\rho u_1'' u_1'' c''} / \rho_0 S_L^2$ from DNS data (—), TDH(—), CC(— —) and New model (—) with x_1 / δ_Z (log scale) for cases A, C and E (1st -3rd column) at $t = 2 \delta_z / S_L, 6 \delta_z / S_L$ and $10 \delta_z / S_L$ (1st -3rd row).

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