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Turbulent kinetic energy transport in head-on quenching of turbulent premixed flames in the context of Reynolds Averaged Navier Stokes simulations

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Abstract

This paper investigates the statistical behaviour of the turbulent kinetic energy transport for moderate values of turbulent Reynolds number Re_t in turbulent premixed flames by using Direct Numerical Simulation (DNS) data in the case of head-on quenching by an isothermal inert wall for different Lewis numbers (i.e. $Le = 0.8$ to 1.2). The magnitudes of turbulent kinetic energy and the terms of its transport equation have been found to increase with a reduction in global Lewis number. The magnitudes of all the terms except the viscous dissipation rate drops sharply near the wall whereas the magnitude of viscous dissipation rate exhibits a sharp increase in the near-wall region. The statistical behaviours of the terms arising from turbulent transport, pressure fluctuation transport, mean pressure gradient, pressure dilatation and viscous dissipation have been analysed by explicit Reynolds averaging of DNS data. It has been found that the viscous dissipation term acts as a major sink for all cases and all locations. The mean pressure gradient acts as the leading order source for all cases. However, the magnitudes of the mean pressure gradient, pressure dilatation and transport terms diminish with increasing Lewis number. Moreover, turbulent flux of kinetic energy has been found to exhibit counter-gradient transport and its extent diminishes with increasing Lewis number as a result of the weakening of flame normal acceleration. Detailed physical explanations have been provided for the observed behaviour of the turbulent kinetic energy transport. Existing models for the unclosed terms have been modified for accurate prediction of the corresponding terms extracted from DNS data especially in the near-wall region.

Keywords: Turbulent kinetic energy, dissipation rate, turbulent premixed flames, Reynolds

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1. Introduction

Flame-wall interaction has important implications on structural integrity, thermal efficiency and unburned hydrocarbon emission in engineering application such as in Spark Ignition (SI) engines. The presence of the wall reduces flame wrinkling and eventually leads to flame quenching [1, 2, 3, 4, 5, 6, 7, 8, 9, 10]. In comparison to the vast body of literature on non-reacting turbulent wall-bounded flows (see [11, 12] and references therein), limited effort [1, 2, 3, 4, 5, 6, 7, 8, 9, 10] has been directed to fundamental understanding of near-wall dynamics within turbulent reactive flows using Direct Numerical Simulation (DNS) data. Turbulent flow modelling for both reactive and non-reacting flows requires the knowledge of turbulent kinetic energy as the unclosed Favre-averaged Reynolds stresses $\overline{\rho u_i'' u_j''}$ are usually modelled using a gradient hypothesis (i.e. $-\overline{\rho u_i'' u_j''} = \mu_t (\partial \tilde{u}_i / \partial x_j + \partial \tilde{u}_j / \partial x_i) - (2\delta_{ij}/3) [\mu_t (\partial \tilde{u}_k / \partial x_k) + \tilde{\rho} \tilde{k}]$) with a turbulent eddy viscosity μ_t where ρ is the fluid density, u_j is the j^{th} component of velocity, and the Favre average and Favre fluctuation of a general quantity q are given by $\tilde{q} = \overline{\rho q} / \tilde{\rho}$ and $q'' = q - \tilde{q}$ respectively. The turbulent eddy viscosity μ_t can be expressed in terms of turbulent kinetic energy $\tilde{k} = \overline{\rho u_i'' u_i''} / 2\tilde{\rho}$ and its dissipation rate $\tilde{\varepsilon} = \overline{\mu (\partial u_i'' / \partial x_j \partial u_j'' / \partial x_i) / \tilde{\rho}}$ in the context of the $k-\varepsilon$ model [13, 14] with μ being the dynamic viscosity. The transport of turbulent kinetic energy in the vicinity of wall has been analysed in detail for non-reacting isothermal flows in turbulent boundary layers using DNS data (e.g. Ref.[15]), but the analysis of $\tilde{k}$ transport in the vicinity of the wall for turbulent premixed flames is yet to be reported in existing literature. The presence of heat release in premixed flames may lead to additional turbulence generation due to flame normal acceleration [16, 17], which may also have significant influences on the turbulent kinetic energy transport in premixed flame-wall interaction. Karlovitz [16] hypothesized the flame-generated turbulence, which was subsequently explained analytically by Bray and Libby [17] who linked this effect with the mean velocity gradient. Moreau and Boutier [18] experimentally confirmed the analytical results by Bray and Libby [17]. Subsequently, Bray *et al.* [19], Borghi and Escudie [20] and Chomiak and Nisbet [21] experimentally demonstrated that the preferential acceleration of lighter burned products over heavier unburned reactants due to flame-induced mean pressure gradient is responsible for flame-generated turbulence. The roles of fluctuating pressure gradient on the turbulent kinetic energy transport for premixed flames have been discussed by Kuznetsov [22] and Strahle [23]. Zhang and Rutland [24] carried out DNS

30 of statistically planar flames and analysed the effects of pressure related terms in the turbulent
 kinetic energy transport equation. Nishiki *et al.* [25] used DNS data to model the flame induced
 effects on the unclosed terms of the turbulent kinetic energy equation in the corrugated flamelets
 regime of premixed turbulent combustion [26]. Chakraborty *et al.* [27] compared the statistical
 behaviour of the turbulent kinetic energy transport between the corrugated flamelets and thin
 35 reaction zones regimes of premixed combustion based on DNS data. A rise of the turbulent kinetic
 energy within the flame brush is likely to occur under certain conditions where the effects of the
 mean pressure gradient and pressure dilatation dominate over the effects of viscous dissipation
 [27]. This situation is more likely to happen in the corrugated flamelets regime, whereas both
 turbulent kinetic energy and its dissipation rate are more likely to decay monotonically through
 40 the flame brush due to weaker mean pressure gradient and pressure dilatation terms than the
 viscous dissipation in the thin reaction zones regime [26]. Furthermore, Chakraborty *et al.* [28]
 demonstrated that the global Lewis number (i.e. $Le = \alpha/D$ is the ratio of thermal diffusivity to
 mass diffusivity) has a significant influence on the turbulent kinetic energy transport, and that the
 effects of flame-generated turbulence strengthen with decreasing Le . It is worth noting that all the
 45 previous analyses [24, 25, 27, 28] on the turbulent kinetic energy transport in turbulent premixed
 flames have been carried out for flows away from the wall. However, the turbulent kinetic energy
 transport in wall-bounded premixed flames is yet to be analysed in detail. Furthermore, the models
 for the additional terms, which appear only in the turbulent kinetic energy transport equation for
 premixed flames, were proposed for flows away from the wall and it remains to be assessed if these
 50 models remain valid in the near-wall region during flame quenching. The present analysis addresses
 this gap in existing literature. Here the turbulent kinetic energy transport and its modelling in
 the near-wall region have been analysed based on three-dimensional DNS of head-on quenching
 of statistically planar turbulent premixed flames by isothermal inert walls for different values of
 Damköhler, Karlovitz and Lewis number Le ($0.8 - 1.2$) in order to analyse the turbulent kinetic
 55 energy transport statistics in the near-wall region. In this respect the specific objectives of this
 paper are:

- To analyse the statistical behaviour of turbulent kinetic energy $\tilde{k}$ and the unclosed terms of
 its transport equation in the near-wall region for head-on quenching of turbulent premixed
 flames.

- To discuss the modelling implications of the unclosed terms of the turbulent kinetic energy $\tilde{k}$ transport equation in the near-wall region based on *a-priori* analysis of DNS data.

2. Mathematical background

Three-dimensional DNS simulations with detailed chemistry are still extremely expensive for a detailed parametric analysis [29]. Thus, a single-step Arrhenius-type irreversible chemical reaction is adopted for current analysis. The chemical composition field for premixed flame is often represented by a reaction progress variable $c = (Y_{R0} - Y_R)(Y_{R0} - Y_{R\infty})$ with Y_R being a reactant mass fraction and the subscripts 0 and ∞ are denoted as the quantities in the unburned and fully burned gases respectively. By definition, c increases monotonically from $c = 0$ in the unburned gas to $c = 1.0$ in the fully burned gas.

The transport equation for the turbulent kinetic energy $\tilde{k} = \overline{\rho u_i'' u_i''} / 2\bar{\rho}$ is in the following form [24, 25, 27, 28]:

$$\begin{aligned} \frac{\partial(\bar{\rho}\tilde{k})}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_j\tilde{k})}{\partial x_j} = & \underbrace{-\overline{\rho u_i'' u_j''} \frac{\partial \tilde{u}_i}{\partial x_j}}_{T_1} - \underbrace{\overline{u_i''} \frac{\partial \bar{p}}{\partial x_i}}_{T_2} + \underbrace{\overline{p' \frac{\partial u_k''}{\partial x_k}}}_{T_3} \\ & + \underbrace{\overline{u_i'' \frac{\partial \tau_{ij}}{\partial x_j}}}_{T_4} - \underbrace{\overline{\frac{\partial (p' u_i'')}{\partial x_i}}}_{T_5} - \underbrace{\overline{\frac{\partial (\frac{1}{2} \rho u_i'' u_k'' u_k'')}{\partial x_i}}}_{T_6} \end{aligned} \quad (1)$$

where the viscous stress tensor is defined as $\tau_{ij} = \mu (\partial u_i / \partial x_j + \partial u_j / \partial x_i) - (2/3) \mu \delta_{ij} (\partial u_k / \partial x_k)$. The term $T_1 = -\overline{\rho u_i'' u_j''} \partial \tilde{u}_i / \partial x_j$ represents the production/destruction of turbulent kinetic energy by the mean velocity gradient [24, 25, 27, 28]. The term $T_2 = -\overline{u_i''} \partial \bar{p} / \partial x_i$ is known as the mean pressure gradient term [24, 25, 27, 28]. The term $T_3 = \overline{p' \partial u_k'' / \partial x_k}$ arises due to the correlation between pressure and dilatation rate fluctuations and is referred to as the pressure dilatation term [24, 25, 27, 28]. The combined effects of molecular diffusion and viscous dissipation of turbulent kinetic energy are described by $T_4 = \overline{u_i'' \partial \tau_{ij} / \partial x_j}$. The term $T_5 = -\overline{\partial (p' u_i'') / \partial x_i}$ and $T_6 = -\overline{\partial (\rho u_i'' u_k'' u_k'') / \partial x_i}$ represent transport of turbulent kinetic energy by pressure fluctuations and turbulent velocity

fluctuations respectively. The term T_4 can alternatively be written as [25, 27, 28]:

$$T_4 = \overline{u_i'' \frac{\partial \tau_{ij}}{\partial x_j}} = -\bar{\rho} \tilde{\varepsilon} + \underbrace{\left[u_i'' \frac{\partial}{\partial x_k} \left(\mu \frac{\partial u_k''}{\partial x_i} \right) - \frac{2}{3} u_i'' \frac{\partial}{\partial x_i} \left(\mu \frac{\partial u_k''}{\partial x_k} \right) \right]}_{T_V} + \frac{\partial}{\partial x_j} \left(\mu \frac{\partial \tilde{k}}{\partial x_j} \right) \quad (2)$$

70 The statistical behaviours of $T_1 - T_6$ in the near-wall region will be analysed in Section 4 of this paper.

3. Numerical implementation

The simulations have been carried out by a DNS code SENGa [30] which solves standard conservation equations of mass, momentum, energy and species for compressible reacting flows in non-dimensional form. A rectangular box of dimensions $70.6\delta_Z \times 35.2\delta_Z \times 35.2\delta_Z$ has been taken for the simulation domain where $\delta_Z = \alpha_{T0}/S_L$ is the Zel'dovich flame thickness with α_{T0} and S_L being the thermal diffusivity of the unburned gas and the unstrained laminar burning velocity respectively. The simulation domain has been discretized using a uniform Cartesian grid of $512 \times 256 \times 256$, which ensures that there are 10 grid points across the thermal flame thickness $\delta_{th} = (T_{ad} - T_0)/\text{Max}|\nabla \hat{T}|_L$, where $\hat{T}$, T_0 and T_{ad} are the dimensional instantaneous, unburned gas and adiabatic flame temperatures respectively. The left hand side of the domain boundary in the x_1 -direction (i.e. $x_1 = 0$) is taken to be a no-slip isothermal wall with temperature $T_W = T_0$ and zero mass flux is enforced in the wall normal direction. The boundary opposite to the isothermal wall is taken to be partially non-reflecting. The boundary conditions are specified using the Navier Stokes Characteristic Boundary Conditions (NSCBC) technique [31]. The rest of the domain boundaries in x_2 and x_3 directions are taken to be periodic. A 10th order central difference scheme is used for spatial differentiation of internal grid points but the order of differentiation decreases gradually to a one-sided 2nd order scheme at the non-periodic boundaries [30]. The time advancement is carried out by using an explicit third-order low storage Runge-Kutta scheme [32].

90 A steady unstrained planar laminar premixed flame solution is used to initialise the reactive field so that the $T = (\hat{T} - T_0)/(T_{ad} - T_0) = 0.9$ isosurface remains at a distance $20\delta_Z$ away from the wall. This allows for enough time for the flame to evolve before interacting with the

wall. The turbulent fluctuating velocity field is initialised using a homogeneous isotropic field of turbulent velocity fluctuations, which is generated using a pseudo-spectral method [33] following the Batchelor-Townsend Spectrum [34], 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 (i.e. $t_e = L_{11}/u'$ where L_{11} is the longitudinal integral length scale and u' is the root-mean-square (rms) turbulent velocity magnitude) before interacting with the flame.

The initial values of normalised 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 $\rho_0 u' L_{11}/\mu_0$ where ρ_0 and μ_0 are the unburned gas density and viscosity respectively. An increase in the numerical value of Re_t by a factor of almost 2.35 is obtained if the integral length scale $l = \tilde{k}^{3/2}/\tilde{\epsilon}$ is used. The turbulent Reynolds number values used here are comparable to the values used in the previous analyses [24, 25, 27, 28] which concentrated on the turbulent kinetic energy transport in turbulent premixed flames. The same range of turbulent Reynolds number was used in the past to analyse the effects of Re_t on turbulent scalar flux [35], Flame Surface Density [36] and Scalar Dissipation Rate [37] closures. Table 1 indicates 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 Zeldovich number $\beta = E_{ac}(T_{ad} - T_0)/RT_{ad}^2$ are taken to be 6.0 (i.e. $\tau = 6.0$ and $\beta = 6.0$) where E_{ac} and R are the activation energy and the gas constant respectively. These values are representative of iso-octane-air mixture with unburned gas temperature $T_0 \approx 325.0K$ and equivalence ratio of 1.10 under atmospheric pressure. The simulations for turbulent cases have been carried out up to a time when the maximum, mean and minimum values of wall heat flux assume identical values following the flame quenching. The simulation time remains different from one case to another 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 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

125 $u_\tau = \sqrt{\tau_w/\rho}$, 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 current analysis, all the Reynolds/Favre averaged quantities are evaluated by ensemble averaging the quantity in question in the transverse direction (i.e. over $x_2 - x_3$ plane) at a given x_1 location. The statistical convergence has been assessed by comparing the results using full and half of available sample sizes. In all cases satisfactory level of statistical convergence has been obtained, and the results based on full sample size will be presented in the next section for the sake of conciseness.

4. Results and discussion

135 4.1. Flame-turbulence interaction

The distributions of non-dimensional temperature $T = (\hat{T} - T_0)/(T_{ad} - T_0)$ at the central $x_1 - x_2$ plane for cases A, C and E are shown in Fig. 1 at three time instants (i.e. $t = 2\delta_Z/S_L, 4\delta_Z/S_L$ and $6\delta_Z/S_L$) for $Le = 0.8, 1.0$ and 1.2 . The cases B and D are not shown explicitly in this and subsequent figures due to qualitative similarities between cases A and B, and between cases D and E. It has been shown in Ref. [9] that the distributions of c and T are qualitatively similar for cases A and B (D and E) (interested readers are referred to Figs. 1 and 2 of Ref. [9]) and thus the cases B and D are not explicitly shown here for the sake of conciseness. Furthermore, the qualitative similarity in behaviour between cases A and B (cases D and E) can be seen from Table 2. A comparison for A, C and E provides an overview of flame-turbulence interaction for this database.

145 The same approach was also adopted in previous publications without any lack of generality in the past [10, 35, 36, 37]. The contours of $c = 0.1$ to 0.9 (from left to right) in steps of 0.2 are shown in Fig. 1 by white lines. In all cases the flame is kept $20\delta_Z$ away from the wall (i.e. $x_1 = 0$ location), but the quenching initiates earlier for cases with higher values of u'/S_L because in these cases the flame elements reach closer to the wall at an earlier time due to greater extent of flame wrinkling (see Fig. 1). This tendency strengthens further for small values of Le as the flame wrinkling away from the wall increases with decreasing Le . The reactants diffuse at a higher rate into the reaction zone than the rate at which heat diffuses out for the flames with $Le < 1$, which leads to concurrent

occurrence of high temperature and reactant concentration in the reaction zone, and just opposite behaviour is observed for $Le > 1$ flames. Table 2 lists the normalised values of turbulent flame speed S_T/S_L (where $S_T = (\rho_0 A_p)^{-1} \int_V \dot{\omega} dV$, $\dot{\omega}$ is the reaction rate of reaction progress variable and A_p is the projected area in the direction of flame propagation) and the normalised turbulent flame surface area A_T/A_L (where $A = \int_V |\nabla c| dV$ is the flame surface area, and the values in turbulent and laminar flames are shown by subscripts T and L, respectively). It can be seen from Table 2 that both A_T/A_L and S_T/S_L increase initially with time (i.e. $t \leq 2\delta_Z/S_L$) due to an increase in flame wrinkling as a result of flame-turbulence interaction, but once the flame quenching is initiated both A_T/A_L and S_T/S_L exhibit decaying trends with time (e.g. $t > 4\delta_Z/S_L$, see also Fig. 3). Table 2 further shows that both A_T/A_L and S_T/S_L assume high values for small Le and/or high u'/S_L cases when the flame is away from the wall (e.g. see $t \leq 2\delta_Z/S_L$ in Fig. 3), and this behaviour is in good agreement with several previous analyses [28, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51]. However, the cases with small Le and/or high values of u'/S_L exhibit smaller values of A_T/A_L and S_T/S_L than in the cases with high values of Le and/or small values of u'/S_L at later times (e.g. $t > 4\delta_Z/S_L$) because by then the flame is in more advanced stage of quenching in the cases with small Le and/or high u'/S_L than in the cases with high Le and/or small u'/S_L .

4.2. Distributions of turbulent kinetic energy $\tilde{k}$ and its dissipation rate $\tilde{\varepsilon}$

The variations of $\tilde{k}$ and $\tilde{\varepsilon}$ in the wall normal direction for cases A, C and E are shown in Fig. 2 for different time instants. The corresponding $\tilde{c}$ and $\tilde{T}$ distributions in the wall normal direction are shown in Fig. 3. It can be seen from Fig. 3 that the distributions of $\tilde{c}$ and $\tilde{T}$ for the $Le = 1.0$ cases are identical to each other when the flame is away from the wall but these distributions become increasingly different from each other as the flame approaches the wall. A similar behaviour has been observed for the distributions of c and T in Fig. 1. The difference in boundary condition at the wall (i.e. Dirichlet boundary condition for temperature, whereas Neumann boundary condition for reaction progress variable) is responsible for the difference between c and T . Thus, $\tilde{T}$ remains 0 (i.e. unburned gas temperature) at the wall, whereas $\tilde{c}$ at the wall (i.e. $x_1 = 0$) increases as the quenching progresses due to zero gradient condition at the wall. The inequality of mass and thermal diffusion gives rise to the inequality between $\tilde{c}$ and $\tilde{T}$ (and also for c and T) for non-unity Lewis number flames even when the flame is away from the wall.

The magnitude of $\tilde{k}$ is found to increase with increasing u'/S_L , as expected. A comparison

between Figs 2 and 3 reveals that both $\tilde{k}$ and $\tilde{\varepsilon}$ decay across the flame brush. Moreover, turbulent kinetic energy decays significantly in the near-wall region (i.e. $x_1/\delta_Z < Pe_{min}$) due to strong viscous action where $Pe_{min} = X_{min}/\delta_Z$ is the minimum wall Peclet number with X_{min} being the minimum wall normal direction of the $T = 0.9$ isosurface [1, 9]. The minimum Peclet number Pe_{min} for turbulent flames remains about the same as the corresponding laminar value $(Pe_{min})_L$ for $Le = 1.0$ and 1.2 but Pe_{min} for turbulent $Le = 0.8$ flames has been found to be smaller than $(Pe_{min})_L$. The minimum Peclet number for laminar head-on quenching $(Pe_{min})_L$ for $Le = 1.0$ is found to be 2.83, which are consistent with previous experimental [52, 53, 54] and computational findings [1]. However, $(Pe_{min})_L$ is found to increase with decreasing Le (i.e. $(Pe_{min})_L = 3.09$ (2.75) for $Le = 0.8$ (1.2)) [9]. The rate of thermal diffusion is smaller than the rate of mass diffusion for the $Le < 1.0$ cases, and thus the unburned reactants from the vicinity of the wall diffuse at a higher rate than the rate of propagation of isotherms towards the wall. Consequently, $(Pe_{min})_L$ in the $Le < 1$ case is greater than the corresponding laminar flame value for $Le = 1.0$. It can be seen from Fig. 1 that the high temperature zones in the turbulent $Le = 0.8$ flames are associated with the zones which are convex towards the reactants where simultaneous strong focussing of reactants and weak defocussing of heat may lead to super-adiabatic temperatures and very high rates of burning. These flame fingers for the turbulent $Le = 0.8$ case, due to their high localised burning rate, can come closer to the wall than the corresponding laminar flame and lead to $(Pe_{min})_L > Pe_{min}$. Interested readers are directed to Ref. [9] for further discussion on the Lewis number dependence of wall Peclet number (i.e. normalised quenching distance) and wall heat flux. Lai and Chakraborty [9] parameterised the minimum Peclet number for turbulent flames as: $Pe_{min} = \Psi = (Pe_{min})_L[erf(8 - 6.0Le) + 1]/2$, which will subsequently be used for the modelling purpose in this paper.

The variation of $\tilde{\varepsilon}$ with x_1/δ_Z in Fig. 2 shows that the high values of $\tilde{\varepsilon}$ are obtained in the near-wall region (i.e. $x_1/\delta_Z < Pe_{min}$). The magnitudes of turbulent kinetic energy and its dissipation rate decrease by a large margin, as the flame quenching progresses. Furthermore, it can be seen from Fig. 2 that the magnitudes of $\tilde{k}$ and $\tilde{\varepsilon}$ increase with decreasing global Lewis number Le . It is useful to analyse the statistical behaviours of the unclosed terms of the turbulent kinetic energy transport equation (see Eq. 1) to explain the variation of $\tilde{k}$ in the near-wall region.

4.3. Statistical behaviour of turbulent kinetic energy transport

The variations of the terms $T_1 - T_6$ in the wall normal direction are shown in Fig. 4. The mean velocity gradient term $T_1 = -\overline{\rho u_1'' u_1''} \partial \tilde{u}_1 / \partial x_1$ acts as a sink (i.e. negative term) for all cases because both $\overline{\rho u_1'' u_1''}$ and $\partial \tilde{u}_1 / \partial x_1$ remain positive throughout the flame brush. The magnitude T_1 becomes negligible in the near-wall region (i.e. $x_1 / \delta_Z < (Pe_{min})_L$). The magnitude of the Reynolds stress $\overline{\rho u_1'' u_1''}$ decays close to the wall due to viscous actions which lead to the decay of the magnitude of T_1 . The quantity $\partial \tilde{u}_1 / \partial x_1$ represents the resolved dilatation rate in the context of RANS of statistically planar flames, and its magnitude increases with decreasing Le due to stronger thermal expansion effects for smaller values of global Lewis number as a result of enhanced burning rate [28, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51]. Thus, the magnitude of the sink contribution of T_1 increases with decreasing Le . The viscous dissipation term T_4 remains the dominant sink in all locations, even at the near-wall region. The large magnitude of the dissipation rate of turbulent kinetic energy $\tilde{\epsilon}$ in the near-wall region (i.e. see Fig. 2) is responsible for the high magnitude of T_4 (see Eq. 2). The mean pressure gradient term T_2 acts as a leading order source within the flame brush away from the wall where the pressure gradient depends mainly on the density variation within the flame. The flame normal acceleration tends to induce a negative mean pressure gradient (i.e. $\partial \bar{p} / \partial x_1 < 0$) across the flame brush. A high rate of heat release in flames with small values of Le gives rise to strengthening of flame normal acceleration effects with decreasing global Lewis number. This leads to an increase in the magnitude of the negative mean pressure gradient $\partial \bar{p} / \partial x_1$ with decreasing Le . The term $\overline{u_1''}$ can be expressed as: $\overline{u_1''} \sim (\rho_0^{-1} - \rho_\infty^{-1}) \overline{\rho u_1'' c''} / \bar{\rho}$ [25, 27, 28] (where ρ_∞ is the burned gas density), and thus the behaviour of the turbulent scalar flux $\overline{\rho u_1'' c''}$ affects the behaviour of T_2 . Furthermore, the turbulent scalar flux $\overline{\rho u_1'' c''}$ exhibits predominantly counter-gradient transport (i.e. $\overline{\rho u_1'' c''} > 0$ where $\partial \tilde{c} / \partial x_1 > 0$ in all cases considered here, which along with predominantly negative values of $\partial \bar{p} / \partial x_1$ gives rise to the positive contribution of the mean pressure gradient term T_2 . The magnitude of T_2 decreases significantly as the flame approaches the wall due to reduced magnitude of $\partial \bar{p} / \partial x_1$ as a result of flame quenching and diminishing magnitude of $\overline{u_1''}$ due to damping of turbulence in the near-wall region.

The pressure dilatation term T_3 and the pressure transport term T_5 exhibit both positive and negative values. The magnitudes of T_3 and T_5 remain comparable for all cases irrespective of the value of Le . The negative values of the pressure dilatation term T_3 are consistent with the previous

DNS based findings [28], but are in contrast to the models proposed by Zhang and Rutland [24] and Nishiki *et al.* [25], which only predict positive values of T_3 proportional to $\tau^2 S_L^3 \rho_0 / \delta_{th}$. Thus improved models for the pressure dilatation term T_3 will be necessary. The effects of dilatation rate and pressure fluctuations due to heat release in the near-wall region weaken with the progress of flame quenching and consequently the magnitudes of T_3 and T_5 in the near-wall region (i.e. $x_1/\delta_Z < (Pe_{min})_L$) decrease with time. As the effects of dilatation rate and heat release induced pressure fluctuation strengthen with decreasing Le , the magnitudes of T_3 and T_5 also increase with decreasing global Lewis number. The magnitude of the turbulent transport term T_6 has been found to be smaller than the other terms in Eq. 1. It is evident from Fig. 4 that the sink contribution of T_4 remains the leading order contributor to $\tilde{k}$ transport in the near-wall region and its magnitude overwhelms the positive contributions of other source terms, and thus, $\tilde{k}$ decays significantly in the near-wall region.

4.4. Modelling of the mean velocity gradient term T_1

The closure of T_1 depends on the modelling of the Reynolds stress $(-\overline{\rho u_i'' u_j''})$, which is usually modelled using the Boussinesq's hypothesis as [11, 12, 13, 14]:

$$\frac{\overline{\rho u_i'' u_j''}}{\bar{\rho}} = -\nu_t \left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) + \frac{2}{3} \delta_{ij} \left(\nu_t \frac{\partial \tilde{u}_k}{\partial x_k} + \tilde{k} \right) \quad (3)$$

where the eddy kinematic viscosity is given by $\nu_t = C_\mu \tilde{k}^2 / \tilde{\epsilon}$ where $C_\mu = 0.09$ is the model constant. According to Eq. 3 the Reynolds stress $\overline{\rho u_1'' u_1''}$ in the direction of mean flame propagation is given by:

$$\frac{\overline{\rho u_1'' u_1''}}{\bar{\rho}} = -\frac{4}{3} \nu_t \frac{\partial \tilde{u}_1}{\partial x_1} + \frac{2}{3} \tilde{k} \quad (4)$$

The variations of $\widetilde{u_1'' u_1''} / S_L^2$ in the wall normal direction for cases A, C and E are shown in Fig. 5 along with the predictions of Eq. 4. It can be seen from Fig. 5 that Eq. 4 tends to underpredict the magnitude of $\widetilde{u_1'' u_1''} / S_L^2$ when the flame is away from the wall, but at later stages of flame-wall interaction Eq. 4 significantly overpredicts $\widetilde{u_1'' u_1''} / S_L^2$. At a given instant of time the flames with higher u' / S_L and smaller values of Le exhibit greater extent of flame-wall interaction, and thus the overprediction of $\widetilde{u_1'' u_1''} / S_L^2$ by Eq. 4 close to the wall is more prominent for case E and for $Le = 0.8$ than the cases with smaller u' / S_L (e.g. case A) and higher Le (e.g. $Le = 1.2$). By the same token,

the underprediction of $\widetilde{u_1'' u_1''}/S_L^2$ by Eq. 4 away from the wall is more prominent for case A and for $Le = 1.2$ than the cases with higher u'/S_L (e.g. case E) and smaller Le (e.g. $Le = 0.8$).

According to Bray-Moss-Libby (BML) analysis [55], which assumes a bi-modal probability density function (PDF) of c , which assumes impulses at $c = 0$ and $c = 1.0$ leads to an alternative expression of $\overline{\rho u_i'' u_j''}$:

$$\frac{\overline{\rho u_i'' u_j''}}{\bar{\rho}} = (1 - \tilde{c})\overline{(u_i' u_j')}_R + \tilde{c}\overline{(u_i' u_j')}_P + \frac{(\overline{\rho u_i'' c''})(\overline{\rho u_j'' c''})}{\bar{\rho}^2 \tilde{c}(1 - \tilde{c})} + O(1/Da) \quad (5a)$$

which leads to:

$$\frac{\overline{\rho u_1'' u_1''}}{\bar{\rho}} = (1 - \tilde{c})\overline{(u_1'^2)}_R + \tilde{c}\overline{(u_1'^2)}_P + \frac{(\overline{\rho u_1'' c''})^2}{\bar{\rho}^2 \tilde{c}(1 - \tilde{c})} + O(1/Da) \quad (5b)$$

where $\overline{(u_1'^2)}_R$ and $\overline{(u_1'^2)}_P$ the conditionally averaged mean-squared velocity fluctuations in the x_1 -direction. The contribution $(1 - \tilde{c})\overline{(u_1'^2)}_R + \tilde{c}\overline{(u_1'^2)}_P$ accounts for the influence of background fluid turbulence and $(\overline{\rho u_1'' c''})^2/[\bar{\rho}^2 \tilde{c}(1 - \tilde{c})]$ is the contribution arising from flame normal acceleration. The last term on right hand side of Eq. 5 originates from the interior of the flame and this contribution remains negligible for high Damköhler number (i.e. $Da \gg 1$) flames. Chakraborty *et al.* [28] modelled the contribution of $(1 - \tilde{c})\overline{(u_1'^2)}_R + \tilde{c}\overline{(u_1'^2)}_P$ by Boussinesq's hypothesis as:

$$(1 - \tilde{c})\overline{(u_1'^2)}_R + \tilde{c}\overline{(u_1'^2)}_P = -\frac{4}{3} \frac{C_\mu}{\sigma_{Le}} \frac{\rho_0 \tilde{k}^2}{\bar{\rho} \tilde{\varepsilon}} \frac{\partial \tilde{u}_1}{\partial x_1} + \frac{2}{3} \tilde{k} \quad (6)$$

where ρ_0 is the unburned gas density and $\bar{\rho} \tilde{\varepsilon}/\rho_0$ the density-weighted dissipation rate which is used here to account for changes in the viscosity with temperature and $\sigma_{Le} = Le^{-1}$ is a turbulent Prandtl number which will be used to account for Lewis number effects. Furthermore, for a presumed bi-modal distribution of reaction progress variable with impulses at $c = 0$ and 1 yields $\overline{\rho c'' c''} = \bar{\rho} \tilde{c}(1 - \tilde{c}) + O(1/Da)$. This enabled Chakraborty *et al.* [28] to propose an alternative model:

$$\frac{\overline{\rho u_1'' u_1''}}{\bar{\rho}} = -\frac{4}{3} \frac{C_\mu}{\sigma_{Le}} \frac{\rho_0 \tilde{k}^2}{\bar{\rho} \tilde{\varepsilon}} \frac{\partial \tilde{u}_1}{\partial x_1} + \frac{2}{3} \tilde{k} + \frac{\overline{\rho u_1'' c''} \overline{\rho u_1'' c''}}{\bar{\rho} \overline{\rho c'' c''}} \quad (7)$$

The predictions of Eq. 7 are also shown in Fig. 5, which shows a better level of agreement with DNS data than the model given by Eq. 4 when the flame is away from the wall. However, the performance of the models given by Eqs. 4 and 7 remain mostly comparable in the near-wall

region. Similar to Eq. 4 the model given by Eq. 7 also overpredicts $\widetilde{u_1''u_1''}$ close to the wall during flame-wall interaction. This over-prediction originates due to simultaneous dampening of $\widetilde{u_1''u_1''}$ and strengthening the magnitude of $\partial\tilde{u}_1/\partial x_1$ close to the wall. This deficiency is addressed here by an adjustment to Eq. 7 in the following manner:

$$\frac{\overline{\rho u_1'' u_1''}}{\bar{\rho}} = Q_1 \left[-\frac{4}{3} \frac{C_\mu}{\sigma_{Le}} \frac{\rho_0 \tilde{k}^2}{\bar{\rho} \tilde{\epsilon}} \frac{\partial \tilde{u}_1}{\partial x_1} + \frac{2}{3} \tilde{k} + \frac{\overline{\rho u_1'' c''} \overline{\rho u_1'' c''}}{\bar{\rho} \overline{\rho c'' c''}} \right] \quad (8)$$

where $Q_1 = 0.5[\text{erf}(x_1/\delta_Z - \Psi) + 1]$ is a damping function such that it asymptotically approaches unity away from the wall (i.e. $x_1/\delta_Z > (Pe_{min})_L$) and thus Eq. 8 becomes identical to Eq. 7. The predictions of Eq. 8 in Fig. 5 reveals that this model does not overpredict $\widetilde{u_1''u_1''}$ in the near-wall region and its performance is comparable to Eq. 7 away from the wall. Thus, Eq. 8 performs better than the other alternative models. It is worth noting that the turbulent scalar flux $\overline{\rho u_1'' c''}$ in Eqs. 7 and 8 is also unclosed and needs modelling. The closure of $\overline{\rho u_1'' c''}$ for head-on quenching of turbulent premixed flames has been addressed elsewhere [56], and thus will not be repeated here.

4.5. Modelling of the mean pressure gradient term T_2

The modelling of the mean pressure gradient term T_2 translates to the modelling of $\overline{u_i''}$. The quantity can be expressed as [25]:

$$\overline{u_i''} = \int_0^1 u_1'' P(c) dc = \int_0^1 \rho u_1'' \frac{P(c)}{\rho} dc \quad (9)$$

where $P(c)$ is the PDF of reaction progress variable. For unity Lewis number flames, the gas density can be expressed as [25]:

$$\frac{1}{\rho} = \frac{(1 + \tau c)}{\rho_0} = \frac{c}{\rho_\infty} + \frac{1 - c}{\rho_0} \quad (10)$$

Substituting Eq. 10 in Eq. 9 leads to the following expression proposed by Nishiki *et al.* [25]:

$$T_2 = -\frac{\tau}{\rho_0} \overline{\rho u_1'' c''} \frac{\partial \bar{p}}{\partial x_1} \quad (11)$$

Chakraborty *et al.* [28] modified the model given by Eq. 11 for non-unity Lewis number flames in the following manner:

$$T_2 = -\frac{\tau}{\rho_0} \left[f \overline{\rho u_1'' c''} + (1 - f) \overline{\rho u_1'' T''} \right] \frac{\partial \bar{p}}{\partial x_1} \quad \text{where } f = 0.5 \quad (12)$$

Figure 6 shows the comparison between the predictions of Eqs. 11 and 12 along with T_2 extracted from DNS for cases A, C and E at different time instants. The mean pressure gradient term T_2 starts from zero at the wall and its magnitude gradually increases toward the coming flame. Both Eqs. 11 and 12 predict T_2 in a satisfactory manner. However, non-negligible values of turbulent scalar flux $\overline{\rho u_1'' c''}$ leads to over-prediction of T_2 in the near-wall region by Eqs. 11 and 12. Therefore, the turbulent scalar flux $\overline{\rho u_1'' c''}$ contribution is required to be damped in the near-wall region. Thus, Eq. 12 is modified here in the following manner:

$$T_2 = -\frac{\tau}{\rho_0} \left[f_w \overline{\rho u_1'' c''} + (1 - f) \overline{\rho u_1'' T''} \right] \frac{\partial \bar{p}}{\partial x_1} \quad \text{where } f_w = 0.5 \exp \left[-2 \left(\tilde{c} - \tilde{T} \right) \right] \quad (13)$$

Equation 13 approaches Eq. 12 away from the wall where $\tilde{c} \approx \tilde{T}$. This can be substantiated from Fig. 6 which shows that Eq. 13 predicts T_2 satisfactorily for both close to and away from the wall.

Moreover, the performance of Eq. 13 remains comparable to Eqs. 11 and 12 away from the wall.

4.6. Modelling of the mean pressure gradient term T_3

Figure 7 presents the variations of the pressure dilatation term T_3 with x_1/δ_Z . It can be seen that the contribution of T_3 changes sign across the flame brush but predominantly assumes positive values when the flame is away from the wall. However, negative contribution of T_3 can be found in the near-wall region as flame approaches the wall in all cases. According to Zhang and Rutland [24] the pressure dilatation term T_3 can be expressed in the following manner:

$$T_3 = p' \frac{\partial u_i''}{\partial x_i} = \frac{1}{V} \int_V p' \frac{\partial u_i''}{\partial x_i} dV = \frac{1}{V} \int_S \int p' \frac{u_i''}{\partial x_i} d\xi dS \quad (14)$$

where dS and dV denote the elemental surface and volume elements, ξ is the local flame normal direction, and $\Sigma = |\nabla c|$ is the generalised Flame Surface Density (FSD) [56]. The pressure dilatation rate term T_3 is given by: $T_3 = \langle I \rangle_s \Sigma$ where I is given by:

$$I = \int_\delta (p - \bar{p}) \left(\frac{du_n}{d\xi} - \frac{\partial \tilde{u}_i}{\partial x_i} \right) d\xi \quad (15)$$

where u_n is the velocity component in the flame normal direction. A one-dimensional analysis of fluid flow in the flame normal direction yields the following relation:

$$p = p_R - \rho_0 u_R (u_n - u_R) \quad (16)$$

the subscript R is used to denote the values in the unburned reactants. Equation 16 yields:

$$\langle I \rangle_s = \langle (p_R - \bar{p})\Delta u \rangle_s - 0.5 \langle \rho_0 u_R (\Delta u)^2 \rangle_s - \langle (p - \bar{p})(\partial \tilde{u}_i / \partial x_i) \delta \rangle_s \quad (17)$$

where δ is a length scale characterising the flame thickness. The pressure drop $(p_R - \bar{p})$ remains positive for positive values of Δu , which leads to a positive contribution of $\langle (p_R - \bar{p})\Delta u \rangle_s$ throughout the flame brush. The second term on the right hand side of Eq. 17 is a negative term. For the unity Lewis number flames the following scalings can be used [24]:

$$\langle (p_R - \bar{p})\Delta u \rangle_s \sim \tau^2 \rho_0 S_L^3; \langle \rho_0 u_R (\Delta u)^2 \rangle_s \sim \tau^2 \rho_0 S_L^3 \quad (18)$$

where $(p_R - \bar{p})$ is scaled with respect to the pressure drop across the laminar flame (i.e. $\tau^2 \rho_0 S_L^3$) and the quantities Δu and $\rho_0 u_R$ are scaled using $\Delta u \sim \tau S_L$ and $\rho_0 u_R \sim \rho_0 S_L$ for the unity Lewis number flames. The last term on the right hand side of Eq. 17 scales in the following manner for the unity Lewis number flames:

$$\langle (p - \bar{p})(\partial \tilde{u}_i / \partial x_i) \delta \rangle_s \sim \tau \rho_0 S_L^3 \left(\frac{U_{mean}}{u'} \right) Da^{-1} \quad (19)$$

Here, $(p - \bar{p})$ and $(\partial \tilde{u}_i / \partial x_i)$ are scaled as $\tau \rho_0 S_L^2$ and U_{mean}/l respectively with U_{mean} being the characteristic mean velocity scale. Thus, the last term on the right hand side of Eq. 17 remains negligible in comparison to the other terms for high Damköhler number Da flames. However, this contribution may not be negligible for low Da flames.

Zhang and Rutland [24] utilised the scalings given by Eq. 18 to model the pressure dilatation term T_3 (stated as PDZ model) in the following manner:

$$T_3 = \frac{1}{2} C_Z \rho_0 S_L^3 \tau^2 \bar{c} \Sigma \quad (20)$$

where C_Z is a model parameter with a value equal to 1.35. Nishiki *et al.* [25] proposed an alternative model (stated as PDN model) as:

$$T_3 = C_N S_L^2 \tau^2 \bar{\omega} \quad (21)$$

where C_N is equal to 0.35 and $\bar{\omega}$ is the mean reaction rate of reaction progress variable. It is worth noting that Eqs. 20 and 21 only predict the positive values of T_3 whereas negative values of T_3 can be observed from Fig. 7. Furthermore, Eqs. 20 and 21 were proposed for unity Lewis number flames. Chakraborty *et al.* [28] proposed a model which take into the consideration of Lewis number effects and the possibility of negative value of T_3 , which is expressed as (i.e. PDC model):

$$T_3 = \bar{\omega} \left[\frac{(1+\tau)\tilde{c}}{(1+\tau\tilde{c})} - \frac{1}{2} \right] [f(Le)\tau S_L]^2 - C_c D_0 \frac{\bar{\omega}}{S_L} \frac{\partial \tilde{u}_k}{\partial x_k} [f(Le)\tau S_L] \quad (22)$$

where $f(Le) = \exp[Le^{-n} - 1]$ with $n = 0.5$ and $C_c = 0.1$ is a model constant. In the derivation of Eq. 22 the quantities $\langle (p_R - \bar{p})\Delta u \rangle_s \Sigma$ and $\langle \rho_0 u_R (\Delta u)^2 \rangle_s \Sigma$ are scaled as:

$$\langle (p_R - \bar{p})\Delta u \rangle_s \Sigma \sim \bar{\omega} \frac{(1+\tau)\tilde{c}}{(1+\tau\tilde{c})} [f(Le)\tau S_L]^2; \quad \langle \rho_0 u_R (\Delta u)^2 \rangle_s \Sigma \sim \bar{\omega} [f(Le)\tau S_L]^2 \quad (23)$$

where $(p_R - \bar{p})$ is scaled as: $(p_R - \bar{p}) \sim \bar{\omega}(1+\tau)\tilde{c}/(1+\tau\tilde{c})\rho_0 u_R \Delta u$ according to Domingo and Bray [57], whereas Δu and $\rho_0 u_R$ are estimated as: $\Delta u \sim f(Le)\tau S_L$ and $\rho_0 u_R \sim \bar{\omega}/\Sigma$ respectively where $f(Le)$ is a function of Lewis number which accounts for strengthening of flame normal acceleration with decreasing Lewis number. The term $\langle (p - \bar{p})(\partial \tilde{u}_i / \partial x_i) \delta \rangle_s \Sigma$ in the PDC model is approximated as:

$$\langle (p - \bar{p})(\partial \tilde{u}_i / \partial x_i) \delta \rangle_s \Sigma = C_{T_3} D_0 \frac{\bar{\omega}}{S_L} \frac{\partial \tilde{u}_k}{\partial x_k} [f(Le)\tau S_L] \quad (24)$$

Both PDZ and PDN models assume a situation where $p_R > \bar{p}$ which associates the pressure drop across the flame brush only due to flame normal acceleration, and it predicts positive values of T_3 . However, it has been demonstrated by Chakraborty *et al.* [28] that the negative values of T_3 is obtained at the flame front location which states $p_R < \bar{p}$. These effects are neglected by the PDZ and PDN models. Both the PDZ and PDN models do not adequately capture the qualitative behaviour of T_3 for all cases considered here and predict the wrong sign close to the wall. The absence of $\bar{\omega}$ in the near-wall region due to flame quenching severely damps the predictions of the PDN and PDC models, whereas T_3 assumes non-negligible magnitude close to the wall. Since, the PDC model provides the best performance among all these models, in terms of qualitative and quantitative agreements with DNS data away from the wall, this model has been considered here

for the modification in the near-wall region:

$$T_3 = \rho_0 S_L \Sigma \left[\frac{(1 + \tau)\tilde{c}}{1 + \tau\tilde{c}} - \frac{1}{2} \exp(1.2\tilde{c}_W) \right] [f(Le)\tau S_L]^2 - C_4 D_0 \rho_0 \Sigma \frac{\partial \tilde{u}_k}{\partial x_k} [f(Le)\tau S_L] \quad (25)$$

The quantity $[(1 + \tau)\tilde{c}/(1 + \tau\tilde{c}) - 1/2]$ in the PDC model plays an important role in the prediction of negative values of T_3 . In the near-wall region, the contribution of $\langle \rho_0 u_R (\Delta u)^2 \rangle_s$ is expected to be greater than the contribution arising from flame normal acceleration because no-slip condition at the wall sets up a stronger $\langle \rho_0 u_R (\Delta u)^2 \rangle_s$ than in a freely propagating flame away from the wall. This aspect is accounted for by the factor $\exp(1.2\tilde{c}_W)$ where $\tilde{c}_W$ is the value of $\tilde{c}$ at the wall and $\exp(1.2\tilde{c}_W)$ becomes identically equal to 1.0 when the flame is away from the wall when $\tilde{c}_W = 0$. Furthermore, $\bar{\omega}$ in the PDC model has been replaced by $\rho_0 S_L \Sigma$, because $\bar{\omega}$ vanishes for $x_1 \delta_Z < Pe_{min}$ due to flame quenching, but Σ assumes non-zero values even at the wall. It can be seen from Fig. 7 that the model given by Eq. 25 satisfactorily predicts T_3 both close to and away from the wall.

4.7. Modelling of the molecular diffusion and dissipation contribution T_4

The variations of T_4 , $\nabla \cdot (\mu \nabla \tilde{k})$, $(-\bar{\rho}\tilde{\epsilon})$ and T_V in the wall normal direction are shown in Fig. 8 for cases A, C and E. Figure 8 shows that $(-\bar{\rho}\tilde{\epsilon})$ remains the major contributor to T_4 and the magnitude of T_V remain smaller than $(-\bar{\rho}\tilde{\epsilon})$ for all cases considered here. The magnitude of T_V remain insignificant in comparison to the magnitudes of $\nabla \cdot (\mu \nabla \tilde{k})$ and $(-\bar{\rho}\tilde{\epsilon})$ in the near-wall region. Moreover, the magnitude of $\nabla \cdot (\mu \nabla \tilde{k})$ remains insignificant in comparison to $(-\bar{\rho}\tilde{\epsilon})$ away from the wall but these contributions become comparable in the near-wall region. The term T_V acts as a sink term, which is consistent with the earlier findings [24, 25, 28]. The magnitudes of T_4 , $\nabla \cdot (\mu \nabla \tilde{k})$, $(-\bar{\rho}\tilde{\epsilon})$ and T_V diminish with time subsequent to flame quenching.

Nishiki *et al.* [25] estimated the order of magnitude of T_V as:

$$T_V = \overline{u_i'' \frac{\partial}{\partial x_k} \left(\mu \frac{\partial u_k''}{\partial x_i} \right)} - \frac{2}{3} \overline{u_i'' \frac{\partial}{\partial x_i} \left(\mu \frac{\partial u_k''}{\partial x_k} \right)} \sim O(-\rho_0 \tau S_L^2 \sqrt{\tilde{k}} \Sigma) \quad (26a)$$

where u_i'' , μ and $\partial u_k''/\partial x_k$ are scaled using $\sqrt{\tilde{k}}$, $\rho_0 S_L \delta_{th}$ and $\tau S_L \Sigma \sim \tau S_L / \delta_{th}$ respectively.

This yields the following model for T_V according to Nishiki *et al.* [25]:

$$T_V = -C_{add} \rho_0 \tau S_L^2 \sqrt{\tilde{k}} \Sigma \quad (26b)$$

where C_{add} is a model constant which is taken to be 0.25. In Eq. 26b the spatial derivative of $\partial u_k''/\partial x_k$ is scaled with respect to δ_{th} . This scaling may not be valid only in the thin reaction zones regime as the effects of dilatation rate is not likely to be confined in a thin region. As a result of better mixing in the thin reaction zones regime it can be assumed that the spatial derivative of $\partial u_k''/\partial x_k$ is scaled with respect to the flame brush thickness which can be scaled using the integral length scale (i.e. $1/|\nabla\tilde{c}| \sim l \sim \tilde{k}^{1.5}/\tilde{\varepsilon}$), which leads to an alternative order of magnitude estimate for T_V :

$$T_V \sim O(-\tilde{\varepsilon}\mu_0\Delta u_s/\tilde{k}\delta_{th}) \quad (26c)$$

where μ_0 is the dynamic viscosity in the reactants and $\partial u_k''/\partial x_k$ is scaled as: $\partial u_k''/\partial x_k \sim \Delta u_s/\delta_{th}$ where Δu_s represents an appropriate slip velocity which is taken to be $\Delta u_s = \tau S_L/Le^r$ (where $r > 0$) as the effects of dilatation rate strengthen with decreasing Lewis number. This suggests that the order of magnitude estimate presented in Eq. 26c can be rewritten as:

$$T_V = -O(\rho_0\tau S_L^2\sqrt{\tilde{k}}\Sigma Le^{-r} Re_t^{-0.5} Da^{-0.5}) \quad (26d)$$

Chakraborty *et al.* [28] utilised Eq. 26d to propose an alternative model:

$$T_V = -C_{VM}\frac{\tilde{\varepsilon}}{\tilde{k}}\mu_0\tau S_L\frac{\tilde{c}^p(1-\tilde{c})^q}{Le^r\delta_{th}} \quad (26e)$$

where $C_{VM} = 0.32$ is a model constant, and $p = 3.33 - 2.45Le$, $q = 0.64 + 0.78Le$ and $r = 3.0$ are the model parameters. The predictions of the models given by Eqs. 26b and 26e are compared to T_V obtained from DNS data in Fig. 9. The model given by Eq. 26b overpredicts the magnitude of T_V away from the wall for cases with high u'/S_L (e.g. case E). By contrast, Eq. 26e satisfactorily predicts the magnitude of T_V in cases A-C but significantly underpredicts the magnitude of T_V in case E when the flame is away from the wall. However, Eq. 26e severely overpredicts the magnitude of T_V close to the wall. The combination of large magnitude of $\tilde{\varepsilon}$ and small value of $\tilde{k}$ reduces the local turbulent Reynolds number $Re_t = \rho_0\tilde{k}^2/\tilde{\varepsilon}\mu_0$ in the near-wall region. Moreover chemical activity weakens due to flame quenching close to the wall, which is expected to be reflected in the drop of local Damköhler number $Da \propto \tilde{k}S_L/\tilde{\varepsilon}\delta_{th}$ in the near-wall region. A comparison between Eqs. 26a and 26c reveals that the prediction of Eq. 26e is likely to yield greater magnitudes of T_V

than Eq. 26b. Here the models given by Eqs. 26a and 26b have been combined to propose the following expression according to the suggestion by Chakraborty *et al.* [27]:

$$T_V = E_3 \left\{ -f(Ka_L).C_{add}\tau\tilde{k}^{1/2}S_L\tilde{\omega} - E_1[1 - f(Ka_L)]C_{VM}\frac{\tilde{\varepsilon}}{\tilde{k}}\mu_0\tau S_L\frac{\tilde{c}^p(1-\tilde{c})^q}{Le_r\delta_L} \right\} \quad (27)$$

where $f(Ka_L) = \exp(-1.92 \times 0.5^{E_2} \times [Ka_L/(1 + Ka_L)]^{1.83})$, $E_1 = 0.5\{erf[x_1/\delta_Z - 0.5\exp(\tilde{c}_W - \tilde{T}_W)\Psi] + 1\}$, $E_2 = 1 - 0.5[erf(x_1/\delta_Z - 10) + 1]$ and $E_3 = \exp[-Le(\tilde{c} - \tilde{T})]$ with $Ka_L = (\tilde{\varepsilon}\delta_{th})^{0.5}S_L^{-1.5}$ being the local Karlovitz number. The function $f(Ka_L)$ increases increasing local Karlovitz number Ka_L which ensures the contribution of Eq. 26b (Eq. 26e) weakens (strengthens) with increasing Ka_L and *vice versa*. The parameter E_1 damps the large magnitude of $(\tilde{\varepsilon}/\tilde{k})$ close to the wall, whereas E_3 damps the overall magnitude of the model expression close to the wall. It can be seen from Fig. 9 that Eq. 27 predicts T_V more satisfactorily than Eqs. 26b and 26e. However, Eq. 27 does not adequately predict T_V at all locations, but the magnitude of T_V remains small in comparison to the leading order contributions of $(-\bar{\rho}\tilde{\varepsilon})$ so the modelling inaccuracies of T_V are unlikely to play an important role in modelling $\tilde{k}$ transport. The dissipation rate $\tilde{\varepsilon}$ needs closure, which beyond the scope of current analysis and will be addressed elsewhere.

4.8. Modelling of the pressure transport term T_5

The pressure transport term T_5 is often stated as:

$$T_5 = -\frac{\overline{\partial(p'u_i'')}}{\partial x_i} = -\overline{u_i''\frac{\partial p'}{\partial x_i}} = -\overline{p'\frac{\partial u_i''}{\partial x_i}} = -\overline{u_i''\frac{\partial p'}{\partial x_i}} - T_3 \quad (28)$$

where the term $-\overline{u_i''\partial p'/\partial x_i}$ is called the fluctuating pressure gradient term. In order to model T_5 , it will be easier to model the fluctuating pressure gradient term $-\overline{u_i''\partial p'/\partial x_i}$, since T_3 as been discussed in the previous section. Launder *et al.* [58] proposed a model (denoted as the PTL model) for $-\overline{u_i''\partial p'/\partial x_i}$ which is given as:

$$-\overline{u_i''\frac{\partial p'}{\partial x_i}} = C_L\overline{\rho u_i''u_j''}\frac{\partial \tilde{u}_i}{\partial x_j} - C_{L2}\bar{\rho}\tilde{\varepsilon} \quad (29)$$

where $C_L = 1.5$ and $C_{L2} = 0.2$ are the model constants. According to Strahle [23] the term $-\overline{u_i''\partial p'/\partial x_i}$ can be modelled as (denoted as the PTS model):

$$-\overline{u_i''\frac{\partial p'}{\partial x_i}} = \frac{1}{2}C_{st}\overline{\rho u_i''u_j''}\frac{\partial \tilde{u}_i}{\partial x_j} \quad (30)$$

where C_{st} is the order of unity. The model proposed by Zhang and Rutland [24] (PTZR) is given by:

$$-u_i'' \frac{\partial p'}{\partial x_i} = \frac{1}{2} \rho_0 S_L^3 \Sigma \tau^3 \frac{(\tilde{c}(1 - \tilde{c}))}{(1 + \tau)} \quad (31)$$

Domingo and Bray [57] provided a model for the quantity $-\overline{u_i'' \partial p / \partial x_i} = T_2 - \overline{u_i'' \partial p' / \partial x_i}$ in the following manner for strict flamelet combustion (i.e. $Da \gg 1$):

$$\begin{aligned} -\overline{u_i'' \frac{\partial p}{\partial x_i}} &= -\frac{\overline{\rho u_i'' c''}}{\bar{\rho}(1 + \tau \tilde{c})} \left[-\frac{\partial \bar{p}_R}{\partial x_i} + (1 + \tau \frac{\partial \bar{p}_P}{\partial x_i}) \right] - \frac{(1 - \tilde{c})}{(1 + \tau \tilde{c})} \overline{u'_{R,i} \frac{\partial p'_R}{\partial x_i}} \\ &\quad - \frac{(1 + \tilde{c})}{(1 + \tau \tilde{c})} \overline{u'_{P,i} \frac{\partial p'_P}{\partial x_i}} + \frac{1}{2} \rho_0 \tau S_L^2 \Sigma < \vec{N} \cdot \vec{M}_i > \frac{\overline{\rho u_i'' c''}}{\bar{\rho}(1 - \tilde{c})} \end{aligned} \quad (32)$$

$$+ 0.35 \rho_0 \tau^2 S_L^3 \Sigma < \vec{N} \cdot \vec{M}_i > < \vec{N} \cdot \vec{M}_i >$$

where the subscripts R and P refer to conditional values in reactants and products respectively, $\vec{N} = -\nabla c / |\nabla c|$ is the local flame normal vector and $\vec{M}_i$ is the component of unit vector describing the mean flame propagation. The value of $< \vec{N} \cdot \vec{M}_j >$ varies between -0.5 to -0.3 in the present cases which is consistent with earlier findings [57]. The conditional values in reactants and products are evaluated using samples corresponding to $0 \leq c \leq 0.1$ and $0.9 \leq c \leq 1.0$ respectively, following previous analyses [28, 57]. The prediction of (Eq. 32– T_2) is referred to as the PTDB model in Fig. 10. Chakraborty *et al.* [28] extended the PTDB model for $Da < 1$ combustion (denoted as the PTNKC model) as:

$$\begin{aligned} -\overline{u_i'' \frac{\partial p'}{\partial x_i}} &= -g \frac{\overline{\rho u_i'' c''}}{\bar{\rho}(1 + \tau \tilde{c})} \left[-\frac{\partial \bar{p}_R}{\partial x_i} + (1 + \tau \frac{\partial \bar{p}_P}{\partial x_i}) \right] - g \frac{(1 - \tilde{c})}{(1 + \tau \tilde{c})} \overline{u'_{R,i} \frac{\partial p'_R}{\partial x_i}} \\ &\quad - g \frac{(1 + \tilde{c})}{(1 + \tau \tilde{c})} \overline{u'_{P,i} \frac{\partial p'_P}{\partial x_i}} + g \frac{1}{2} \rho_0 \tau S_L^2 \Sigma < \vec{N} \cdot \vec{M}_i > \frac{\overline{\rho u_i'' c''}}{\bar{\rho}(1 - \tilde{c})} \\ &\quad + 0.35 g \rho_0 \tau^2 S_L^3 \Sigma < \vec{N} \cdot \vec{M}_i > < \vec{N} \cdot \vec{M}_i > \\ &\quad + (1 - g) C_{1N} \overline{\rho u_i'' u_j''} \frac{\partial \tilde{u}_i}{\partial x_j} - (1 - g) C_{2N} \bar{\rho} \tilde{\varepsilon} + \frac{g \tau}{\rho_0} \left[f \overline{\rho u_i'' c''} + (1 - f) \overline{\rho u_i'' T''} \right] \frac{\partial \bar{p}}{\partial x_i} \end{aligned} \quad (33)$$

where $g = \widetilde{c}''^2 / \tilde{c}(1 - \tilde{c})$ is the segregation factor and $C_{1N} = 1.05$, $C_{2N} = 0.14$ and $f = 0.5$ are the model parameters. The PTDB model is valid for the reactive region in the corrugated flamelets regime whereas the model PTL was suggested for the non-reacting flows. A linear bridging model based on segregation factor $g = \widetilde{c}''^2 / \tilde{c}(1 - \tilde{c})$ is used in the PTNKC model.

Figure 10 presents the variations of $-\overline{u_i'' \partial p' / \partial x_i}$ with x_1 / δ_Z for cases A, C and E. Figure 10 shows the PTNKC model has an advantage over the other alternative models in terms of the prediction of $-\overline{u_i'' \partial p' / \partial x_i}$ from DNS data when the flame is far away from the wall. The PTL and PTS models do not sufficiently capture the qualitative and quantitative behaviours of $-\overline{u_i'' \partial p' / \partial x_i}$, whereas the PTZR and PTDB models to some extent capture the qualitative behaviour of $-\overline{u_i'' \partial p' / \partial x_i}$. It is worth noting that the agreement between the PTZR model and DNS data improves as the flame approaches the wall. The contribution of $(-\bar{\rho}\tilde{\varepsilon})$ in the PTL and PTNKC models is responsible for large negative values in the near-wall region, whereas DNS data shows negligible values of $-\overline{u_i'' \partial p' / \partial x_i}$ close to the wall. Here, the PTKNC and PZR models have been combined here to propose a new model as:

$$\begin{aligned} -\overline{u_i'' \frac{\partial p'}{\partial x_i}} &= -g^* \frac{\overline{\rho u_i'' c''}}{\bar{\rho}(1 + \tau \tilde{c})} \left[-\frac{\partial \bar{p}_R}{\partial x_i} + (1 + \tau \frac{\partial \bar{p}_P}{\partial x_i}) \right] - g^* \frac{(1 - \tilde{c})}{(1 + \tau \tilde{c})} \overline{u'_{R,i} \frac{\partial p'_R}{\partial x_i}} \\ &\quad - g^* \frac{(1 + \tilde{c})}{(1 + \tau \tilde{c})} \overline{u'_{P,i} \frac{\partial p'_P}{\partial x_i}} + g^* \frac{1}{2} \rho_0 \tau S_L^2 \Sigma < \vec{N} \cdot \vec{M}_i > \frac{\overline{\rho u_i'' c''}}{\bar{\rho}(1 - \tilde{c})} \\ &\quad + 0.35 g^* \rho_0 \tau^2 S_L^3 \Sigma < \vec{N} \cdot \vec{M}_i > < \vec{N} \cdot \vec{M}_i > \end{aligned} \quad (34)$$

$$\begin{aligned} &+ \left[(1 - g) C_{1N} \overline{\rho u_i'' u_j''} \frac{\partial \tilde{u}_i}{\partial x_j} - (1 - g) C_{2N} \bar{\rho} \tilde{\varepsilon} \right] f_{err} + \left[0.1 \rho_0 S_L^3 \Sigma \tau^3 \frac{\tilde{c}(1 - \tilde{c})}{(1 + \tau)} \right] (1 - f_{err}) \\ &\quad + \frac{g\tau}{\rho_0} \left[f \overline{\rho u_i'' c''} + (1 - f) \overline{\rho u_i'' T''} \right] \frac{\partial \bar{p}}{\partial x_i} \end{aligned}$$

where g^* and f_{err} are given as:

$$g^* = \exp(\tilde{c}_W - \tilde{T}_W) \left[\frac{\widetilde{c}''^2}{\tilde{c}(1 - \tilde{c})} \right]^{0.5} \left[\text{erf} \left(\frac{x_1}{\delta_Z} - 10 \right) + 1 \right]; \quad f_{err} = 0.5 [\text{erf}(x_1 / \delta_Z - \Psi) + 1] \quad (35)$$

The PTKNC model underpredicts the magnitude of $-\overline{u_i'' \partial p / \partial x_i}$ in the near-wall region due to the negligible value of the segregation factor g in that zone [18, 19]. The $\exp(\tilde{c}_W - \tilde{T}_W)$ dependence

of g^* increases the magnitude of the prediction of the PTDB model as $(\tilde{c}_W - \tilde{T}_W)$ increases as the flame quenching progresses (because $\tilde{c}_W$ remains zero away from the wall but it approaches unity as the flame quenching progresses, whereas $T_W = 0$ at the isothermal wall). The satisfactory performance of the PTZR model in the near-wall region is utilised to add the contribution of $[0.1\rho_0 S_L^3 \Sigma \tau^3 \tilde{c}(1 - \tilde{c})/(1 + \tau)](1 - f_{err})$ in the model expression given by Eq. 35 to provide an accurate prediction in the region given by $x_1/\delta_Z < Pe_{min} = \Psi$. It can be seen in Fig. 10 that Eq. 35 provides the better qualitative and quantitative agreements with DNS data than the other alternative model expressions.

4.9. Modelling of the turbulent transport term T_6

The closure of the turbulent transport term T_6 translates to the modelling of $\overline{\rho u_i'' k} = \overline{\rho u_i'' u_j'' u_j''}/2$, which in turn boils down to the closure of $\overline{\rho u_1'' k} = \overline{\rho u_1'' u_j'' u_j''}/2$ for statistically planar flames. According to Bray-Moss-Libby (BML) analysis [55] one gets:

$$\begin{aligned} \overline{\rho u_1'' k} &= \frac{\overline{\rho u_1'' u_j'' u_j''}}{2} = \bar{\rho} \{ (1 - \tilde{c}) \overline{u'_{1R} k_R} + \overline{\tilde{c} u'_{1P} k_P} + \tilde{c} (1 - \tilde{c}) (\bar{u}_{1P} - \bar{u}_{1R}) (\bar{k}_P - \bar{k}_R) \\ &\quad + \frac{1}{2} \tilde{c} (1 - \tilde{c}) (\bar{u}_{1P} - \bar{u}_{1R})^3 (1 - 2\tilde{c}) \} \end{aligned} \quad (36a)$$

where $\bar{k}_R = \overline{u'_{1R} u'_{1R}}/2$ and $\bar{k}_P = \overline{u'_{1P} u'_{1P}}/2$ are the conditional values of the turbulent kinetic energy in reactants and products respectively. The contribution $\bar{\rho} \{ (1 - \tilde{c}) \overline{u'_{1R} k_R} + \overline{\tilde{c} u'_{1P} k_P} \}$ represents the non-reacting contribution to the unclosed turbulent flux of turbulent kinetic energy. In the case of non-reacting turbulent flows $\overline{\rho u_1'' k}$ is usually modelled using a gradient hypothesis in the following manner [11, 14]:

$$\overline{\rho u_1'' k} = -\bar{\rho} C_{T1} \frac{\tilde{k}^2}{\tilde{\varepsilon}} \frac{\partial \tilde{k}}{\partial x_1} \quad (36b)$$

The same approach can be applied for the closure of the non-reacting contribution $\bar{\rho} \{ (1 - \tilde{c}) \overline{u'_{1R} k_R} + \overline{\tilde{c} u'_{1P} k_P} \}$ as [27, 28]:

$$\bar{\rho} \{ (1 - \tilde{c}) \overline{u'_{1R} k_R} + \overline{\tilde{c} u'_{1P} k_P} \} = -\bar{\rho} C_{T2} \frac{\tilde{k}^2}{\tilde{\varepsilon}} \frac{\partial \tilde{k}}{\partial x_1} \quad (36c)$$

According to BML analysis [55] the slip velocity ($\bar{u}_{1P} - \bar{u}_{1R}$) in Eq. 36a can be expressed as:

$$(\bar{u}_{1P} - \bar{u}_{1R}) = \frac{\overline{\rho u_1'' c''}}{\rho c''^2} \quad (36d)$$

Chakraborty *et al.* [27, 28] modelled the difference in the mean turbulent kinetic energy between products and reactants as:

$$(\bar{k}_P - \bar{k}_R) = -C_{T3} \frac{1}{\Sigma} M_i \frac{\partial \tilde{k}}{\partial x_i} \quad (36e)$$

where $M_i = -(\partial \tilde{c} / \partial x_i) / |\nabla \tilde{c}|$ is the resolved flame normal vector component in the i^{th} direction. Combining Eqs. 36a, 36c, 36d, 36e yields [27, 28]:

$$\overline{\rho u_1'' k} = -\bar{\rho} C_{T2} \frac{\tilde{k}^2}{\tilde{\varepsilon}} \frac{\partial \tilde{k}}{\partial x_1} - C_{T3} \overline{\rho u_1'' c''} \frac{1}{\Sigma} M_i \frac{\partial \tilde{k}}{\partial x_i} + \frac{1}{2(\overline{\rho c''^2})^2} (\overline{\rho u_1'' c''})^3 (1 - 2\tilde{c}) \quad (36f)$$

It is worth noting that the BML analysis assumes a bi-modal probability density function (pdf) of c with impulses at $c = 0$ and $c = 1$ but it has been demonstrated elsewhere [9, 10] that the pdf of c does not remain bi-modal in the near-wall region. Chakraborty *et al.* [28] modified Eq. 36f for the conditions where pdf of c shows a departure from bi-modal distribution in the following manner:

$$\overline{\rho u_1'' k} = -\bar{\rho} C_{T2} \frac{\tilde{k}^2}{\tilde{\varepsilon}} \frac{\partial \tilde{k}}{\partial x_1} - C_{T3} \overline{\rho u_1'' c''} \frac{1}{\Sigma} M_i \frac{\partial \tilde{k}}{\partial x_i} + \frac{1}{2(\overline{\rho c''^2})^2} (\overline{\rho u_1'' c''})^3 (1 - 2\tilde{c}g^s) \quad (36g)$$

where $g = \tilde{c}''^2 / \tilde{c}(1 - \tilde{c})$ is the segregation factor which assumes a value of unity for bi-modal distribution with impulses at $c = 0$ and $c = 1$ and it becomes increasingly smaller than unity for increasing deviation of the pdf of c from a bi-modal distribution. Chakraborty *et al.* [28] suggested

330 $C_{T2} = 0.22$, $C_{T3} = 1.0$ and $s = 2$ for the model parameters.

The predictions of $-\mu_t(\partial \tilde{k} / \partial x_1)$ (where $\mu_t = 0.09\bar{\rho}(\tilde{k}^2 / \tilde{\varepsilon})$), Eqs. 36f and 36g are compared to $\overline{\rho u_i'' k}$ extracted from DNS data in Fig. 11. In non-reacting turbulent flows $\overline{\rho u_1'' u_j'' u_j''} / 2$ is often modelled as $\overline{\rho u_1'' u_j'' u_j''} / 2 = -(\mu_t / \delta_k)(\partial \tilde{k} / \partial x_1)$ using a gradient hypothesis [11, 13, 14]. It has been found that both $\overline{\rho u_1'' u_j'' u_j''} / 2$ and $-\mu_t(\partial \tilde{k} / \partial x_1)$ assume the same sign in the near-wall region (i.e. 335 $0 < x_1 / \delta_Z < (Pe_{min})_L$) in all cases. However, $\overline{\rho u_1'' u_j'' u_j''} / 2$ and $-\mu_t(\partial \tilde{k} / \partial x_1)$ assume opposite signs at some locations within the flame brush when the flame is away from the wall, and this behaviour is more prevalent in the $Le = 0.8$ case than in the $Le \geq 1.0$ cases because the strong flame normal

acceleration in a low Lewis number flame is more likely to overwhelm the effects of turbulent velocity fluctuations to give rise to counter-gradient transport [27, 28]. The effects of flame normal acceleration weaken due to flame quenching, and thus the gradient transport dominates in the near-wall region.

Equations 36f and 36g are more successful in capturing the qualitative behaviour of $\overline{\rho u_1'' k}$ extracted from DNS data than the gradient hypothesis model (i.e. Eq. 36b) when the flame is away from the wall and quantitative agreement with DNS data is marginally better for Eq. 36g than in Eq. 36f. However, in the near-wall region, Eqs. 36f and 36g start to over-predict by large margin, and at the advanced stage of quenching, no models predict the correct sign and magnitude of turbulent flux of kinetic energy $\overline{\rho u_1'' k}$. In order to capture the near-wall behaviour of $\overline{\rho u_1'' k}$ Eq. 36g has been modified here in the following manner:

$$\overline{\rho u_1'' k} = \alpha_4 \left[-\bar{\rho} C_{T2} \frac{\tilde{k}^2}{\tilde{\varepsilon}} \frac{\partial \tilde{k}}{\partial x_1} - C_{T3} \overline{\rho u_1'' c''} \frac{1}{\Sigma} M_i \frac{\partial \tilde{k}}{\partial x_i} + \frac{1}{2(\rho c''^2)^2} (\overline{\rho u_1'' c''})^3 (1 - 2\tilde{c}g^s) \right] \quad (37)$$

where $C_{T3W} = [(-2)^{a_2} \exp(\tilde{c}_W)]^{a_1}$ with $a_1 = 1 - 0.5[\text{erf}(x_1/\delta_Z - \Psi) + 1]$ and $a_2 = 0.5[\text{erf}(\tilde{c}_W - 0.55Le) + 1]$ and $a_4 = 0.5[\text{erf}(x_1/\delta_Z - \exp(-\tilde{c}_W)\Psi) + 1]$. The modification of C_{T3W} allows for dampening of turbulent kinetic energy close to the wall. The model parameter a_2 makes sure that the modification of C_{T3} becomes active only at an advanced stage of quenching and a_1 restricts the region of modification close to the wall. The model parameter a_4 ensures the magnitude of $\overline{\rho u_1'' k}$ is adequately captured. The predictions of Eq. 37 are shown in Fig. 11 which reveals that the predictions of Eq. 37 are in better agreement with $\overline{\rho u_1'' k}$ from DNS than the other model expressions. However, the level of agreement between DNS data and the prediction of Eq. 37 is relatively better for $Le = 1.0$ and 1.2 cases than the $Le = 0.8$ cases. It can be seen from Fig. 11 that Eq. 37 does not adequately capture the qualitative/quantitative behaviour of $\overline{\rho u_1'' k}$ at some instants of time (e.g. at $t = 10\delta_Z/S_L$ for case A and at $t = 2\delta_Z/S_L$ and $6\delta_Z/S_L$ for case E). It has been shown in Fig. 4 that T_6 remains small in comparison to the leading order contributors to turbulent kinetic energy $\tilde{k}$ transport so the modelling inaccuracies of $\overline{\rho u_1'' k}$ may not have a significant role in modelling $\tilde{k}$ transport.

In order to assess the combined influence of all the models proposed here, the net contribution of $(T_1 + T_2 + T_3 + T_4 + T_5 + T_6)$ as obtained from DNS data is compared to the combined modelled prediction of according to Eqs. 8, 13, 25, 27, 34 and 37 in Fig. 12, which shows a satisfactory

agreement between DNS data and model predictions for all Lewis number and turbulent intensities considered here.

5. Conclusions

The statistical behaviour and modelling of the transport of turbulent kinetic energy in the case of head-on quenching of turbulent premixed flames by an isothermal inert wall have been investigated for different values of $u'/S_L, l/\delta_{th}$ and Le under moderate values of Re_t . The turbulent kinetic energy decays significantly in the vicinity of the wall, whereas its dissipation rate increases close to the wall. It has been found that the mean pressure gradient term T_2 remains the leading order source for all cases whereas the viscous contribution T_4 acts as a leading order sink. The contributions arising from mean velocity gradient and turbulent transport (i.e. T_1 and T_5) remain negligible in comparison to the magnitude of the viscous contribution T_4 for all cases considered here. The magnitudes and the strengths of mean pressure gradient and pressure dilatation terms (i.e. T_2 and T_3) decrease with increasing Lewis number due to the weakening of burning rate and flame normal acceleration. The pressure dilatation and pressure transport terms (i.e. T_3 and T_5) have been found to play significant roles in the turbulent kinetic energy transport and the behaviours of T_3 , T_4 , T_5 and T_6 have been found to be significantly affected by the presence of the wall. Furthermore, the turbulent flux of kinetic energy has been found to exhibit counter-gradient behaviour and the extent of counter-gradient transport weakens with increasing Lewis number Le . The existing models for T_3 , T_4 , T_5 and T_6 have been assessed in comparison to the corresponding terms extracted from explicitly Reynolds averaged DNS data and it has been found that the existing models for T_3 , T_4 , T_5 and T_6 need modification in order to provide satisfactory prediction in the vicinity of the wall. Modifications to the existing model expressions which yield satisfactory performance away from the wall have been suggested so that they predict the behaviour of DNS data both away from and close to the wall. It is recognised that the DNS cases considered here have moderate values of turbulent Reynolds number Re_t . However, there also have been several analyses which showed the model parameters for turbulent scalar flux [35], Flame Surface Density [36] and Scalar Dissipation Rate [37] assume asymptotic value at relatively small values of Re_t (for $Re_t \geq 50$) so that the modelling become Reynolds number independent for relatively small values of turbulent Reynolds number. It can indeed be seen from the model expressions given by Eqs. 8, 13, 25, 27, 34 and 37 that they assume asymptotic value for $50 < Re_t < 100$. It can indeed

be seen from Figs. 4–12 that cases C-E behave mostly similarly for a given value of global Lewis
 number. However, these models need further validation based on detailed chemistry DNS data for
 390 higher values of Re_t . Moreover, they need to be implemented in actual RANS code for *a-posteriori*
 assessment, but this is beyond the scope of this paper. In actual RANS simulations, the numerical
 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 expected
 395 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 combustion models and thus
 turbulence 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 kinetic energy transport models and without them, will not be able to
 400 isolate whether the differences in the simulation results arise only due to turbulent kinetic energy
 models or due to kinetic energy dependence of the mean reaction rate and scalar flux closures.
 Some of the aforementioned questions will form the foundation of future research activities.

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Table 1: List of initial simulation parameters and non-dimensional numbers.

Case	A	B	C	D	E
u'/S_L	5.0	6.25	7.5	9.0	11.25
l/δ_{th}	1.67	1.44	2.5	4.31	3.75
Da	0.33	0.23	0.33	0.48	0.33
Ka	8.67	13.0	13.0	13.0	19.5
Re_t	22.0	23.5	49.0	100	110

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.

		A		B		C		D		E		
		$\frac{tS_L}{\delta_Z}$	$\frac{A_T}{A_L}$	$\frac{S_T}{S_L}$	$\frac{A_T}{A_L}$	$\frac{S_T}{S_L}$	$\frac{A_T}{A_L}$	$\frac{S_T}{S_L}$	$\frac{A_T}{A_L}$	$\frac{S_T}{S_L}$	$\frac{A_T}{A_L}$	$\frac{S_T}{S_L}$
$Le = 0.8$	1	1.62	1.61	1.69	1.68	3.5	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	6.7	
	4	2.64	2.62	2.36	2.35	2.69	2.67	2.32	2.3	1.5	1.48	
	6	1.9	1.88	1.7	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	2.9	4.18	4.17	
	2	1.67	1.66	1.6	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	0.5	0.49	0.2	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	
	10	0.17	0.17	1.69	1.68	3.50	3.47	3.26	3.23	5.33	5.29	
$Le = 1.2$	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	2.75	2.74	3.43	3.43	
	4	1.31	1.3	1.28	1.27	1.82	1.81	1.98	1.96	1.57	1.55	
	6	1.3	1.29	1.29	1.28	1.6	1.59	1.51	1.49	1.23	1.22	
	8	1.23	1.22	1.24	1.23	1.12	1.11	0.6	0.6	0.47	0.46	
	10	1.15	1.14	1.14	1.13	0.6	0.6	0.18	0.18	0.1	0.1

Figure 1: Instantaneous non-dimensional temperature 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), white line presents c field from 0.1 to 0.9 with interval of 0.2 from left to right.

Figure 2: Variations of $\tilde{k}/S_L^2$ and $\tilde{\varepsilon} \times \delta_Z/S_L^3$ for cases A, C and E (1st-3rd column) at $t = 2\delta_Z/S_L$ (—), $6\delta_Z/S_L$ (—) and $10\delta_Z/S_L$ (—).

Figure 3: Variations of $\tilde{c}$ and $\tilde{T}$ for cases A, C and E (1st-3rd column) at $t = 2\delta_Z/S_L$ (—), $6\delta_Z/S_L$ (—) and $10\delta_Z/S_L$ (—).

Figure 4: Variations of term T_1 (—), T_2 (—), T_3 (— —), T_4 (—), T_5 (— —) and T_6 (—) 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 terms are non-dimensionalised by $\rho_0 S_L^3/\delta_Z$.

Figure 5: Variations of $\widetilde{u_1''u_1''}/S_L^2$ from DNS data (—) and according to the predictions of Eq.4 (—), Eq.7 (— o —) and Eq.8 (—) 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).

Figure 6: Variations of $T_2 \times \delta_Z / \rho_0 S_L^3$ from DNS (— + —) and according to the predictions of Eq.11 (—), Eq.12 (— o —) and Eq.13 (—) 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).

Figure 7: Variations of $T_3 \times \delta_Z / \rho_0 S_L^3$ from DNS (—) and according to the predictions of PDZ (—), PDN (---), PDC (---) and Eq.25 (—) 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).

Figure 8: Variations of $T_4 \times \delta_Z / \rho_0 S_L^3$ (—), $\nabla \cdot (\mu \cdot \nabla \tilde{k}) \times \delta_Z / \rho_0 S_L^3$ (—), $(-\bar{\rho} \tilde{\epsilon}) \times \delta_Z / \rho_0 S_L^3$ (---) and $T_V \times \delta_Z / \rho_0 S_L^3$ (---) 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).

Figure 9: Variations of $T_V \times \delta_Z / \rho_0 S_L^3$ from DNS data (—), Eq.26ii (—), Eq.26v (— o —) and Eq.27 (—) 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).

Figure 10: Variations of $-\overline{u''_i \partial p' / \partial x_i} \times \delta_Z / \rho_0 S_L^3$ from DNS data (—), PTL (—), PTS (—), PTZR (—), PTDB (—), PTNKC (—) and Eq.34 (—○—) with x_1 / δ_Z 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).

Figure 11: Variations of $\overline{\rho u_1'' k} / \rho_0 S_L^3$ from DNS data (—○—), $(-\mu_t \partial \tilde{k} / \partial x_1) / \rho_0 S_L^3$ (—△—), Eq.36vi (—△—), Eq.36vii (—○—) and Eq.37 (—) 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).

Figure 12: Variations of $(T_1 + T_2 + T_3 + T_4 + T_5 + T_6) \times \delta_Z / \rho_0 S_L^3$ from DNS data (—) and the combined modelled prediction according to Eqs. 8, 13, 25, 27, 34 and 37 (—) 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).