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Full Length Article

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 Renolds 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. $Le = 0.8–1.2$). 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.

1. Introduction

Flame-wall interaction has important implications on structural integrity, thermal efficiency and unburned hydrocarbon emission in engineering applications such as in Spark Ignition (SI) engines. The presence of the wall reduces flame wrinkling and eventually leads to flame quenching [1–10]. In comparison to the vast body of literature on non-reacting turbulent wall-bounded flows (see [11,12] and references therein), limited effort [1–10] 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. $-\overline{\rho u_i'' u_j''} = \mu_t(\partial\tilde{u}_i/\partial x_j + \partial\tilde{u}_j/\partial x_i) - (2\delta_{ij}/3)[\mu_t(\partial\tilde{u}_k/\partial x_k) + \bar{\rho}\tilde{k}]$) with a turbulent eddy viscosity μ_t where ρ is the fluid density, u_j is the jth component of velocity, and the Favre average and Favre fluctuation of a general quantity q are given by $\tilde{q} = \overline{\rho q}/\bar{\rho}$ and $q'' = q - \tilde{q}$ respectively. The turbulent eddy viscosity μ_t can be expressed in terms of turbulent kinetic energy $\tilde{k} = \overline{\rho u_i'' u_i''}/2\bar{\rho}$ and its dissipation rate $\tilde{\varepsilon} = \overline{\mu(\partial u_i''/\partial x_j \partial u_i''/\partial x_j)}/\bar{\rho}$ 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

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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 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 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 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 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 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 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 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]:

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

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 $T_5 = -\partial\overline{(p'u_i'')}/\partial x_i$ and $T_6 = -\partial(\overline{\rho u_i'' u_k'' u_k''}/2)/\partial x_i$ 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]:

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

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 $\delta_{th} = (T_{ad} - T_0)/Max|\nabla\widehat{T}|_L$, where $\widehat{T}, T_0$ 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