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Flame surface density based modelling of head-on quenching of turbulent premixed flames

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Abstract

The near-wall behaviour of the generalised flame surface density (FSD) transport in the context of Reynolds Averaged Navier–Stokes (RANS) simulations has been analysed for different values of global Lewis number using three-dimensional Direct Numerical Simulation (DNS) data of head-on quenching of statistically planar turbulent premixed flames by an isothermal inert wall. It has been found that the statistical behaviour of the FSD based reaction rate closure and the terms of the FSD transport equation are significantly affected by the presence of the wall and by the global Lewis number. The near-wall predictions of the standard FSD based mean reaction rate closure and existing sub-models for the unclosed terms of the FSD transport equation have been found to be inadequate based on *a-priori* DNS assessment, and modifications to these models have been suggested so that the predictions of modified models for reaction rate closure and FSD transport remain satisfactory, both close to the wall and away from it over a wide range of global Lewis number.

Keywords: Flame surface density (FSD); Reynolds averaged Navier–Stokes simulations (RANS); Direct numerical simulation (DNS); Head-on quenching; Lewis number

1. Introduction

Direct Numerical Simulation (DNS) contributed significantly to the fundamental understanding of combustion but relatively limited effort has been directed to the analysis of wall-bounded reacting flows [1–7]. Poinsot et al. [3] conducted two-dimensional DNS simulations of "head-on quenching" (HOQ) of turbulent premixed flames, and reported a significant modification of the

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vorticity field within the flame front due to the presence of a wall. Bruneaux et al. [4,5] conducted three-dimensional incompressible DNS simulations of a "sidewall quenching" (SWQ) configuration for a premixed flame in a channel flow configuration. The data obtained from the simulations by Bruneaux et al. [4] was used to analyse a flame surface density (FSD) based reaction rate closure [5]. The near-wall behaviour of a V-flame anchored in a channel flow with isothermal walls was investigated by Alshalaan and Rutland [1,6] and Gruber et al. [7]. Alshalaan and Rutland [6] analysed the near-wall statistics of FSD as well as turbulent scalar transport and wall heat flux.

The FSD quantifies the flame surface area per unit volume of the flame [8], and is often used for the mean chemical reaction rate closure in turbulent premixed flames for both Reynolds Averaged Navier–Stokes (RANS) [9–14] and Large Eddy Simulations (LES) [15–22]. The FSD can either be modelled using an algebraic expression [9,15,17,21] or by solving a modelled transport equation [10–14,16,18,19,22]. The current analysis will focus on the RANS modelling of FSD based mean reaction rate closure in the near-wall region alongside the modelling of the unclosed terms in the transport equation for the generalised FSD (i.e. $\Sigma_{gen} = \overline{|\nabla c|}$ [15], where c is the reaction progress variable and the over-bar denotes Reynolds averaging operation). The case considered is HOQ of statistically planar turbulent premixed flames by an inert isothermal wall for different values of global Lewis number Le (i.e. ratio of thermal diffusivity to mass diffusivity). It is worth noting that most LES simulations reduce to RANS in the near-wall region so that the present analysis will also be relevant to LES. The effects of turbulent Reynolds number Re_t and global Lewis number Le on the statistical behaviour of Σ_{gen} away from the wall have been investigated in a number of recent studies [11–14], which indicated that the qualitative behaviour of the FSD is unaffected by Re_t, but that the relative contributions of the unclosed terms of the FSD Σ_{gen} transport equation are affected to some extent. By contrast, Le may influence both the qualitative and quantitative behaviour of the unclosed terms [11–13]. Furthermore, the conventional FSD based closure for the mean reaction rate ($\overline{\dot{\omega}} = \rho_0 S_L \Sigma_{gen}$ with the unburned gas density ρ_0, and the unstrained laminar burning velocity S_L) is likely to undepredict (overpredict) $\overline{\dot{\omega}}$ for flames with $Le < 1$ ($Le > 1$) respectively [13]. Although the near-wall behaviour of FSD based closures has been addressed in the past [5,6], the effects of turbulence intensity and Le on near-wall FSD modelling of FSD have not yet been considered. This paper addresses this gap by analysing three-dimensional DNS data of HOQ of statistically planar turbulent premixed flames by an inert isothermal wall.

2. Mathematical background

The chemical mechanism is simplified in this study by a single-step Arrhenius-type reaction in order to permit extensive parametric analysis. Several FSD based analyses [5,6,9–22] have already been carried out using single step chemistry, and some of these closures have been demonstrated to be successful in capturing experimental observations [20–22]. Furthermore, the usage of simple chemistry allows for the analysis of Lewis number effects in isolation, which was followed in several previous analyses (see [11,13] and references therein). Detailed chemistry and transport, on the other hand, would lead to an accurate description of wall quenching for the specific set of parameters, but not for general cases. Previous analyses [3,23,24] demonstrated that experimentally obtained wall heat flux and quenching distance [25–27] can be accurately predicted using simple chemistry.

A reaction progress variable $c = (Y_{R0} - Y_R)/(Y_{R0} - Y_{R\infty})$ is defined based on a suitable reactant mass fraction Y_R where the subscripts 0 and ∞ denote the values in the fresh and burned gas, respectively. In RANS, the progress variable transport takes the following form:

$$\partial(\bar{\rho}\tilde{c})/\partial t + \partial\left(\bar{\rho}\tilde{u}_j\tilde{c}\right)/\partial x_j = \overline{\dot{\omega}} + \overline{\nabla\cdot(\rho D\nabla c)} - \partial\left(\overline{\rho u_j'' c''}\right)/\partial x_j \quad (1)$$

Here u_j denotes the jth component of the velocity vector, ρ and D are density and diffusivity of the progress variable respectively, and $\tilde{\varphi} = \overline{\rho\varphi}/\bar{\rho}$ and $\varphi'' = \varphi - \tilde{\varphi}$ are the Favre-mean and -fluctuation of a general quantity φ respectively. The combined reaction rate and molecular diffusion term can be modelled as: $\overline{\dot{\omega}} + \overline{\nabla\cdot(\rho D\nabla c)} = \overline{(\rho S_d)}_s\Sigma_{gen}$ where $\overline{(\varphi)}_s = \overline{\varphi|\nabla c|}/\overline{|\nabla c|}$ denotes surface averaging [15] and $S_d = (Dc/Dt)/|\nabla c|$ is the local displacement speed. For unity Lewis number flames the model $\overline{(\rho S_d)}_s \approx \rho_0 S_L$ is often applied [13,16,21,22]. The transport equation for Σ_{gen} takes the following form [10–14,16,18,19,22]:

$$\begin{aligned}\partial\Sigma_{gen}/\partial t + \partial\left(\tilde{u}_j\Sigma_{gen}\right)/\partial x_j &= \underbrace{-\partial\left\{\left[\overline{(u_i)}_s - \tilde{u}_i\right]\Sigma_{gen}\right\}/\partial x_i}_{T_1-turbulent\ transport} \\ &+ \underbrace{\overline{\left((\delta_{ij} - N_iN_j)\partial u_i/\partial x_j\right)}_s\Sigma_{gen}}_{T_2-strain\ rate} \\ &\underbrace{-\partial\left[\overline{(S_dN_i)}_s\Sigma_{gen}\right]/\partial x_i}_{T_3-propagation} + \underbrace{\overline{(S_d\partial N_i/\partial x_i)}_s\Sigma_{gen}}_{T_4-curvature}\end{aligned} \quad (2)$$

Here $\vec{N} = -\nabla c/|\nabla c|$ is the local flame normal vector. The terms $T_1 - T_4$ are unclosed and thus need modelling. The near-wall modelling of $T_1 - T_4$ will be addressed in Section 4 of this paper.