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A-priori direct numerical simulation assessment of sub-grid scale stress tensor closures for turbulent premixed combustion

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ABSTRACT

The fidelity of large eddy simulations (LES) depends heavily on the closures of the sub-grid scale (SGS) stress tensor but most existing models have been proposed for non-reacting isothermal flows. However, the flame normal acceleration due to chemical heat release significantly affects turbulent flow statistics including the statistical behaviour of SGS stresses within flames but limited effort has been directed to the assessment of the SGS stress tensor closures in turbulent premixed combustion. In the present analysis, the closures of the SGS stress tensor have been *a-priori* assessed with respect to explicitly filtered direct numerical simulation (DNS) data of freely propagating turbulent premixed flames with a range of different values of turbulence intensities and the integral length scale to flame thickness ratios. A variety of scale similarity models has been considered in addition to the well-known static and dynamic Smagorinsky models. Further, a more recent development by Anderson and Domaradzki (2012) has been extended for compressible flows and included in this analysis. Detailed physical explanations have been provided for the observed model performances.

1. Introduction

Turbulent combustion modelling with the large eddy simulation (LES) potentially has advantages over traditional methods due to its ability to resolve large-scale turbulent structures. Subject to the assumptions of low Mach number and unity Lewis number, the temperature and the mass fractions of the reactive species can be uniquely expressed with the help of a reaction progress variable c, which takes the value zero in the unburned reactants and unity in the fully burned products. The Favre-filtered transport equation for the progress variable c can be written as:

$$\frac{\partial \bar{\rho}\tilde{c}}{\partial t} + \frac{\partial}{\partial x_i}(\bar{\rho}\tilde{u}_i\tilde{c}) = -\frac{\partial}{\partial x_i}(\overline{\rho u_i c} - \bar{\rho}\tilde{u}_i\tilde{c}) + \overline{\frac{\partial}{\partial x_i}\left(\rho D \frac{\partial c}{\partial x_i}\right)} + \dot{\omega}_c \quad (1)$$

where ρ, u_i and D denote the gas density, ith component of velocity vector and the progress variable diffusivity respectively. The two terms on the right hand side of Eq. (1) which need to be modelled correspond to the sub-grid turbulent scalar flux $F_i^{sgs} = \overline{\rho u_i c} - \bar{\rho}\tilde{u}_i\tilde{c}$ and the filtered flame front displacement term (i.e. $\overline{\nabla \cdot (\rho D \nabla c) + \dot{\omega}_c}$). The density weighted momentum conservation equation has the form:

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

where ν is the kinematic viscosity. The SGS stress tensor is given by $\tau_{ij}^{SGS} = \overline{\rho u_i u_j} - \bar{\rho}\tilde{u}_i\tilde{u}_j$. The particular modelling challenge in a turbulent premixed flame arises from the fact that the SGS model should be able to capture also the gas-dynamic expansion [1,2]. Indeed it can be shown [3] that in the limit of thin flames the probability density function (PDF) of the progress variable c assumes a bimodal distribution and under these conditions the turbulent scalar flux takes the following form:

$$F_i^{sgs} \approx \bar{\rho}\tilde{c}(1-\tilde{c})\left[\overline{(u_i)_P} - \overline{(u_i)_R}\right] \quad (3)$$

where $\overline{(u_i)_P}$ and $\overline{(u_i)_R}$ are the conditionally filtered velocities in products and reactants respectively. The density of the products is smaller than the density of the reactants and therefore, considering the mass conservation through a steady planar flame, this can lead to $\overline{(u_i)_P} > \overline{(u_i)_R}$ and hence $F_i^{sgs} > 0$. This result cannot be predicted from classical gradient hypothesis closure. Focusing next on momentum transport it is argued, that an expression for the SGS stress tensor may be obtained in the following manner subject to the assumption of the presumed bi-modal sub-grid PDF of c with impulses at

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$c = 0.0$ and 1.0 [3,4]:

$$\tau_{ij}^{SGS} \approx \bar{\rho}(1-\tilde{c})[\overline{(u_i\,u_j)}_R - \overline{(u_i)}_R\ \overline{(u_j)}_R] + \bar{\rho}\tilde{c}[\overline{(u_i\,u_j)}_P - \overline{(u_i)}_P\ \overline{(u_j)}_P] + \bar{\rho}\tilde{c}(1-\tilde{c})[\overline{(u_i)}_P - \overline{(u_i)}_R][\overline{(u_j)}_P - \overline{(u_j)}_R] \quad (4)$$

where $[\overline{(u_i\,u_j)}_R - \overline{(u_i)}_R\ \overline{(u_j)}_R\ ]$ and $[\overline{(u_i\,u_j)}_P - \overline{(u_i)}_P\ \overline{(u_j)}_P]$ are the conditionally filtered SGS stresses in reactants and products respectively. The third term on the right hand side of Eq. (4) indicates the contribution of the velocity jump across the flame brush arising from chemical heat release. It is worth noting that this contribution to the SGS stress tensor vanishes in both unburned (i.e. $\tilde{c} = 0.0$) and burned (i.e. $\tilde{c} = 1.0$) gases. Thus, the magnitude and the sign of the stress depend on the relative magnitudes of the conditional velocities and on the conditional SGS stresses $[\overline{(u_i\,u_j)}_R - \overline{(u_i)}_R\ \overline{(u_j)}_R]$ and $[\overline{(u_i\,u_j)}_P - \overline{(u_i)}_P\ \overline{(u_j)}_P]$. It is important to note, that the subsequent analysis does not assume an infinitely thin reaction front. The theory of Bray et al. [4] is only mentioned here in order to present the theoretical explanation of the occurrence of counter-gradient behaviour of sub-grid stresses. From the foregoing it can be expected that the commonly used Smagorinsky model, relying on the Boussinesq assumption, will not be able to satisfactorily predict the SGS stresses in turbulent premixed flames. Indeed Pfadler et al. [2] demonstrated its unsatisfactory performance based on direct measurements of the density weighted stress tensor. Although several publications deal with the modelling of the SGS scalar flux F_i^{sgs} in reacting flows (see e.g. [5,6] and references therein), only limited effort has been directed to the assessment of sub-grid scale (SGS) stress tensor closures in turbulent premixed combustion [2] which is the focus of this work.

The closures of sub-grid stresses also interact with the closures of other unclosed terms and numerical schemes in actual LES simulations. Thus, it is not straightforward to assess the performances of the sub-grid scalar stress in isolation. Together with the fact that counter-gradient behaviour of SGS stresses is not well documented in the literature, the *a-priori* analysis performed in this work is of interest on its own following the philosophy of several previous analyses [2,7-14].

The rest of the paper is organised as follows. The DNS database used for the current analysis is briefly introduced in the next section. This is followed by a summary of the SGS stress models considered for the current analysis. Following this, the results will be presented and subsequently discussed. Modelling implications of the present findings are highlighted next in a separate section. The conclusions are drawn and main findings are summarised in the final section of this paper.

2. DNS database

In the present analysis, the closures of SGS stress tensor have been *a-priori* assessed with respect to the explicitly filtered simple chemistry based direct numerical simulation (DNS) data of freely propagating statistically planar turbulent premixed flames. The physical mechanisms responsible for gradient/counter gradient stresses (or transport) are dependent on the competition between the turbulent velocity fluctuation and the velocity jump across the flame brush due to heat release. Thus, the qualitative behaviour of SGS stresses will not be different even if one uses complex instead of single step chemistry. The DNS database has been explicitly filtered using a Gaussian filter kernel using seven different filter widths from $\Delta \approx 0.4\ \delta_{th}$ where the flame is almost resolved, up to $\Delta \approx 2.8\ \delta_{th}$ where the flame becomes fully unresolved and Δ is comparable to the integral length scale. The initial values of normalised root mean square turbulent velocity fluctuation u'/S_L, the ratio of turbulent integral length scale to flame thickness l/δ_{th}, Damköhler number $Da = lS_L/\delta_{th}u'$ and Karlovitz number $Ka = (u'/S_L)^{3/2}(l/\delta_{th})^{-1/2}$ are provided in Table 1

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	8.65	13.0	13.0	13.0	19.5

where $\delta_{th} = (T_{ad} - T_0)/Max|\nabla\hat{T}|_L$ is the thermal flame thickness with $\hat{T}$ being the dimensional temperature and the subscript 'L' refers to the unstrained laminar planar flame quantities.

Table 1 indicates that the cases A, C and E (B, C and D) have the same values of Da (Ka). Standard values are chosen for Prandtl number Pr and ratio of specific heats γ (i.e. $Pr = 0.7$ and $\gamma = 1.4$). The flame Mach number $Ma = S_L/\sqrt{\gamma RT_0}$, heat release parameter $\tau = (T_{ad} - T_0)/T_0$ and Lewis number Le are taken to be 0.014, 4.5 and 1.0 respectively. Despite the limitations, inherent to DNS studies, a number of analyses by others based on 3D simple chemistry in canonical configurations with either similar or smaller value of turbulent Reynolds number contributed significantly to the fundamental understanding of turbulent combustion in the last 10 years [11,15-20]. Furthermore, the range of turbulent Reynolds number used in this database is comparable to the well-known experimental database of Bunsen burner flames by Kobayashi et al. [21].

It is worth noting that the flame-turbulence interaction takes place under decaying turbulence for all cases in Table 1, where it is standard practice to choose the simulation time such that $t_{sim} \geq Max(t_f, t_c)$ where $t_f = l/u'$ is the initial eddy turn-over time and $t_c = \delta_{th}/s_L$ is the chemical time scale. This ensures that the final result is independent of initialisation of chemistry and turbulent flow field. In all cases statistics were extracted after one chemical time scale t_c, which corresponds to a time equal to $2.0t_f$ in case D, $3.0t_f$ in cases A, C and E, and $4.34t_f$ for case B respectively. The data is taken from a single frame when the turbulent kinetic energy evaluated over the whole domain and global burning rate were not changing rapidly with time. It has been shown in Chakraborty et al. [22], where the database is described in detail, that results remain qualitatively similar halfway through the simulation. The present simulation time is either comparable to or greater than that used in several previous DNS studies [15,17,23-26] by several other authors that have contributed significantly to the fundamental understanding and modelling of turbulent combustion.

Instantaneous views of isosurfaces for cases A, C and E when the statistics were extracted (i.e. $t = \delta_{th}/S_L$) are shown in Fig. 1. It is evident that the extent of flame wrinkling increases with increasing u'/S_L. For the sake of brevity, results will mostly be shown for cases A, C and E. The cases B and D follow the trends demonstrated by cases A and E respectively.

3. Subgrid scale stress closures

The most conventional SGS model is the Smagorinsky model, which relies on the hypothesis, that the energy transfer from the resolved scale to the SGS is analogous to molecular mechanisms represented by the diffusion term [27]. As for incompressible flow one can take the point of view that the isotropic part of the SGS stresses, i.e. the term involving $-\frac{1}{3}\tau_{kk}^{SGS}\delta_{ij}$, can be added to the filtered pressure. The Smagorinsky model is then given by the expression:

$$\tau_{ij}^{SSM} = -\bar{\rho}\nu_t 2\left(\widetilde{S}_{ij} - \frac{1}{3}\widetilde{S}_{kk}\delta_{ij}\right)\ \nu_t = (C_s\Delta)^2\left|\widetilde{S}_{ij}\right|,$$
$$\widetilde{S}_{ij} = \frac{1}{2}\left(\frac{\partial\widetilde{u}_i}{\partial x_j} + \frac{\partial\widetilde{u}_j}{\partial x_i}\right),\ \left|\widetilde{S}_{ij}\right| = \sqrt{2\,\widetilde{S}_{ij}\widetilde{S}_{ij}} \quad (5)$$