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Benchmark solutions

A-priori Direct Numerical Simulation assessment of models for generalized sub-grid scale turbulent kinetic energy in turbulent premixed flames

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ABSTRACT

The fidelity of Large Eddy Simulation (LES) in the context of turbulent premixed combustion modelling depends on the complex coupling between turbulence and chemical reactions occurring at the unresolved scale. Although LES of combustion systems is becoming increasingly popular, the closures for sub-grid scale (SGS) stresses have mostly been derived assuming constant density flows. Similar to the unclosed scalar flux, the behaviour of the SGS stresses depends on the balance between heat release and turbulence, and it has been shown recently that counter-gradient transport (CGT) can occur for the stress tensor when the isotropic part of the stress tensor is not properly accounted for. This leads to a negative correlation between the predictions obtained from an eddy viscosity type model and the stresses obtained from Direct Numerical Simulation (DNS). In the present work the modelling of the isotropic part of the stress tensor, closely related to the generalised sub-grid scale kinetic energy, is considered in detail. To this end the interplay between SGS dilatation effects and unresolved velocity fluctuations is analysed using *a-priori* DNS analysis of turbulent, statistically planar flames with different values of global Lewis number and heat release parameter. Well-known models for generalised sub-grid scale kinetic energy have been assessed in the context of turbulent premixed combustion and detailed physical explanations for their behaviour have been provided. Further, the effects of SGS dilatation rate on the anisotropy of the SGS stresses have been highlighted using a variant of the Lumley triangle.

1. Introduction

Large Eddy Simulation (LES) is considered to be a promising technique for flows featuring unsteady, large coherent structures. Despite increasing popularity of combustion LES, the closures for sub-grid scale (SGS) stresses for constant density flows are usually used although they do not adequately capture the gas-dynamic expansion in turbulent premixed flames [1,2]. The filtered momentum conservation equation is given as:

$$\frac{\partial \bar{\rho}\widetilde{u}_i}{\partial t} + \frac{\partial\left(\bar{\rho}\widetilde{u}_i\widetilde{u}_j\right)}{\partial x_j} = -\frac{\partial\left(\overline{\rho u_i u_j} - \bar{\rho}\widetilde{u}_i\widetilde{u}_j\right)}{\partial x_j} + \frac{\partial}{\partial x_j}\bar{\rho}\ \tilde{\nu}\left(\left(\frac{\partial \widetilde{u}_j}{\partial x_i} + \frac{\partial \widetilde{u}_i}{\partial x_j}\right) - \frac{2}{3}\frac{\partial \widetilde{u}_k}{\partial x_k}\delta_{ij}\right) - \frac{\partial \bar{p}}{\partial x_i} \quad (1)$$

where ρ, u_i and ν denote the gas density, ith component of velocity vector and kinematic viscosity respectively. The filtering operation is given by: $\overline{Q(\boldsymbol{x})} = \int Q(\boldsymbol{x}-\boldsymbol{r})G(\boldsymbol{r})d\boldsymbol{r}$, where $G(\boldsymbol{r}) = (6/\pi\Delta^2)^{3/2}\exp(-6\ \boldsymbol{r}\cdot\boldsymbol{r}\ /\Delta^2)$ is the Gaussian filter kernel, Δ is the filter width and $\widetilde{Q}\ = \overline{Q\rho}\ /\ \overline{\rho}$ denotes Favre filtering. The SGS stress tensor is given by $\tau_{ij}^{SGS} = \overline{\rho u_i u_j} - \bar{\rho}\widetilde{u}_i\widetilde{u}_j$ [3], and the isotropic part of the SGS stresses, i.e. the term involving $-\frac{1}{3}\tau_{kk}^{SGS}\delta_{ij}$, is often added to the filtered pressure for incompressible flows. The relevance of modelling the isotropic part of the SGS stresses is discussed in some detail in reference [4]. The most popular closure for τ_{ij}^{SGS} is the static Smagorinsky model (SSM), which is given below where $\widetilde{S_{ij}} = (\partial\widetilde{u}_i/\partial x_j + \partial\widetilde{u}_j/\partial x_i)/2$ and $|\widetilde{S_{ij}}| = \sqrt{2\ \widetilde{S_{ij}}\widetilde{S_{ij}}}$:

$$\tau_{ij}^{SSM} = -2\bar{\rho}(C_s\Delta)^2\left|\widetilde{S_{ij}}\right|\left(\widetilde{S_{ij}} - \widetilde{S_{kk}}\delta_{ij}/3\right) \quad (2)$$

The constant C_s is either set to $C_s \approx 0.18$ in the static model version (SSM) or can be determined in a dynamic manner (see Ref. [3] for details). Pfadler et al. [2] demonstrated the Smagorinsky model's unsatisfactory performance based on direct measurements of the density-weighted stress tensor. Klein et al. [4] re-

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cently showed that counter-gradient transport (CGT) for the stress tensor is obtained if the isotropic part of the stress tensor is not properly accounted for. The behaviour of the SGS stresses depends on the balance between heat release and turbulence [4] and the competition between these effects will be analysed in this work by means of *a-priori* DNS analysis of statistically planar flames with different global Lewis numbers Le (i.e. ratio of thermal to mass diffusivities) and heat release parameters $\tau = (T_{ad} - T_0)/T_0$ where T_{ad} and T_0 are the adiabatic flame and unburned gas temperatures respectively.

An explicit model (i.e. YOS model) for the isotropic part of the SGS stress tensor has been suggested by Yoshizawa [5]: $\tau_{kk}^{YOS} = 2\, C_I \bar{\rho}\ \Delta^2 |\widetilde{S_{ij}}|^2$. Yoshizawa [5] recommended a value of $C_I \approx 0.089$ whereas Moin et al. [6] reported a value of C_I ranging from 0.0025 to 0.009. This spread of C_I arises to some extent due to the fact that some studies used a mixed model where the scale-similarity part has a contribution to the diagonal SGS stress components [7]. All these aforementioned studies have been conducted in the context of non-reacting flows. Klein et al. [4] demonstrated that satisfactory results could only be obtained for the dynamic evaluation of C_I using the formula $C_I = \langle L_{kk} M \rangle / \langle M^2 \rangle$ instead of $C_I = \langle L_{kk} \rangle / \langle M \rangle$ [6], in combination with an averaging conditional on $\tilde{c}$. Here, M is defined as: $M = 2\hat{\bar{\rho}}\ \ \hat{\Delta}^2 |\widehat{\widetilde{S_{ij}}}|^2 - 2\widehat{\bar{\rho}\ \Delta^2 |\widetilde{S_{ij}}|^2}$ and $L_{kk} = \widehat{\bar{\rho}\tilde{u}_k\tilde{u}_k} - \widehat{\bar{\rho}\tilde{u}_k}\widehat{\bar{\rho}\tilde{u}_k}/\hat{\bar{\rho}}$ is the Leonard stress [6]. Depending on the turbulence intensity and the LES filter width, values of C_I in the range 0.1-0.2 were found within the flame brush [4], which is considerably larger than the values for isothermal flows reported in the literature. In this work C_I will be globally determined based on a least-squares fit between the modelled and exact stresses obtained from DNS data. Although several analyses (Refs. [8,9] and references therein) deal with the LES modelling of the SGS scalar fluxes, limited effort has been directed to the assessment of SGS stress tensor closures in turbulent premixed combustion [2], and in particular to the modelling of the isotropic part of the stress tensor, which is the focus of this work. The quantity τ_{kk}^{SGS} is closely related to the generalized SGS kinetic energy formally introduced by Germano in the context of constant density flows as [10]: $k^{gsgs} = \frac{1}{2}\tau_{kk}^{SGS}/\bar{\rho}$. For completeness, it is worth mentioning that k^{gsgs} is equal to the SGS kinetic energy $k^{sgs} = \frac{1}{2}\ \overline{u'_{\Delta i} u'_{\Delta i}}$ (where $u'_{\Delta i} = u_i - \overline{u_i}$) , if the filter is a Reynolds operator, which is generally not the case [3]. Besides the modelling of the isotropic part of the stress tensor, k^{gsgs} is also used in different contexts. The velocity fluctuation $u'_{\Delta} = \sqrt{2k^{gsgs}/3}$ represents an important input to many combustion models. Exemplarily, it determines the turbulent flame speed in the G-equation approach [11], it enters the efficiency function in the artificially thickened flame approach [12] and it also affects the wrinkling factor in Flame Surface Density based modelling [13,14]. Furthermore k^{gsgs} is often used to assess the degree of resolution of a LES simulation [15,16]. The main objectives of the present analysis are to: (a) assess existing models for τ_{kk}^{SGS} based on *a-priori* analysis of DNS data for statistically planar turbulent flames with different Le and τ, and (b) provide detailed explanations for the observed behaviour.

The rest of the paper will be organized as follows. The information pertaining to mathematical background and numerical implementation will be provided in the next section. This will be followed by the presentation of results and their discussion. The main findings will be summarized and conclusions will be drawn in the final section of this paper.

2. Mathematical background and numerical implementation

The DNS database considered here was used previously in several studies [8,9,17–23]. It consists of five statistically planar flames with $Le = 0.34$ (case A), 0.6 (case B), 0.8 (case C), 1.0 (case D) and 1.2 (case E). The heat release parameter $\tau = (T_{ad} - T_0)/T_0$ for these cases is taken to be 4.5. An additional case (case F) is considered to analyse the effects of τ, where τ has been set to $\tau = 3.0$ and Le is taken to be 1.0. Standard values of Prandtl number $Pr = 0.7$, Zel'dovich number $\beta_Z = 6.0$ and ratio of specific heats $\gamma_g = 1.4$ were considered for the present analysis. The initial values of the ratio of the root-mean-square turbulent velocity fluctuation and unstrained laminar burning velocity u'/S_L and the integral length scale to thermal flame thickness ratio l/δ_{th} are taken to be 7.5 and 2.5 respectively (i.e. $u'/S_L = 7.5$ and $l/\delta_{th} = 2.5$) in all cases, where $\delta_{th} = (T_{ad} - T_0)/\max|\nabla\hat{T}|_L$ is the thermal flame thickness. The initial values of Damköhler $Da = lS_L/u'\delta_{th}$ and Karlovitz $Ka = (u'/S_L)^{3/2}(l/\delta_{th})^{-1/2}$ numbers are 0.33 and 13.0 respectively. All cases considered here represent the thin reaction zones regime [24] combustion.

The values of u'/S_L and l/δ_{th} used here remain comparable to several previous analyses [25–29] for *a-priori* DNS modelling. Furthermore, the models proposed based on *a-priori* DNS analyses using this database [22,23] have been found to be in good agreement with *a-posteriori* assessments based on actual LES simulations [30,31]. It is worth noting that the findings of this paper are also valid for the database used in Ref. [4] which deals with different values of turbulent Reynolds number Re_t. Furthermore, it is discussed in the Appendix A1 that all findings reported in this paper remain both qualitatively and quantitatively valid for an additional unity Lewis number case with considerably higher values of Re_t and scale separation l/δ_{th}. This provides the confidence in the findings of the present analysis which has been conducted for a moderate dynamic range in favour of an extensive parametric study in terms of Lewis number, heat release parameter, and filter width.

The physical mechanisms responsible for the competing effects of heat release and turbulence on τ_{kk}^{gsgs} can be captured using simplified chemistry. Therefore a single step irreversible chemical mechanism has been considered here. For all cases the simulation domain size was taken to be $24.1\delta_{th} \times 24.1\delta_{th} \times 24.1\delta_{th}$, which was discretised using a uniform Cartesian mesh of 230^3 grid points. High order finite-difference (10th order for the internal grid points and one-sided 2nd order scheme at non-periodic boundaries) and 3rd order low storage Runge-Kutta schemes are used for spatial differentiation and explicit time advancement respectively. The boundary conditions in the mean flame propagation direction (aligned with negative x_1-direction) are taken to be partially non-reflecting, whereas boundaries in transverse directions are taken to be periodic.

The turbulent velocity fluctuations are initialised using a homogeneous isotropic incompressible velocity field. The reacting flow field is initialised by a steady planar unstrained premixed laminar flame solution. In all cases flame-turbulence interaction takes place under decaying turbulence and all non-dimensional numbers mentioned before have to be understood as initial values here and in the remainder of the text. By the time statistics were extracted the value of u'/S_L in the unburned gas ahead of the flame decayed by about 50% of its initial value, whereas the value of l/δ_{th}in the fresh gas increased by about 1.7 times. The simulation time $t_{sim} = 3.34l/u' \approx \delta_{th}/S_L$ is comparable to several previous DNS studies which focused on the modelling of turbulent premixed combustion [25,27–29,32,33]. The data is taken from a single frame where turbulent kinetic energy and the global burning rate were not changing rapidly with time as shown in [11]. Moreover, it was shown there that the results remain qualitatively similar halfway through the simulation.

For this analysis, the DNS data has been explicitly filtered using a Gaussian filter kernel. Results will be presented from $\Delta \approx 0.4\ \delta_{th}$ where the flame is almost resolved, up to $\Delta \approx 2.8\ \delta_{th}$ where the