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Scale similarity based models and their application to subgrid scale scalar flux modelling in the context of turbulent premixed flames

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ABSTRACT

The performance of a variety of scale similarity (SS) type models for closure of sub-grid scalar flux in the context of Large Eddy Simulations (LES) of premixed turbulent combustion has been assessed. In addition to the well-known SS models, a more recent development by Anderson and Domaradzki (2012) is included in the analysis and also further model extensions and improvements are discussed. The work is based on a priori analysis of two Direct Numerical Simulation (DNS) databases of freely propagating turbulent premixed flames with a range of different Lewis and turbulent Reynolds numbers. Depending on the balance between the effects of flame normal acceleration due to heat release and the effects of turbulent velocity fluctuations, as well as the filter size, the subgrid-scalar flux exhibits both local gradient and counter-gradient transport which presents a considerable modelling challenge. The assessment is based on a correlation analysis and on the magnitude of the model expressions conditional on the Favre averaged reaction progress variable in comparison to the value obtained from DNS. Despite the fact that most of the models have been developed in the context of momentum transport in non-reactive flows they show either comparable or better performance in comparison to more conventional models used for reactive scalar flux closure. It is found that some models are sensitive to the test filter width and recommendations are provided in this regard. Further it is observed that the use of a Favre test filter substantially increases the correlation strength in direction of mean flame propagation where effects of heat release are most pronounced.

1. Introduction

Closure of the turbulent scalar flux such as enthalpy or species concentration is one of the main issues in modelling turbulent premixed combustion. Assuming a single-step chemistry and a unity Lewis number (=thermal diffusivity/mass diffusivity) the mass fractions of the reactive species and the non-dimensional temperature in a premixed flame can be expressed using a single variable c assuming the values $c=0$ on the reactant side and $c=1$ in the fully burned products. The corresponding transport equation takes the following form (Peters 2000):

$$\frac{\partial \rho c}{\partial t} + \nabla \cdot (\rho \boldsymbol{u} c) = \nabla \cdot (\rho D \nabla c) + \dot{\omega}_c \tag{1}$$

Here $\rho, \boldsymbol{u}, D$ and $\dot{\omega}_c$ denote density, velocity, progress variable diffusivity and reaction rate respectively. The Large Eddy Simulation (LES) filtering operation of a quantity Q is defined by $\overline{Q(\boldsymbol{x})} = \int Q(\boldsymbol{x}-\boldsymbol{r})G(\boldsymbol{r})d\boldsymbol{r}$ where $G(r)$ is a filter kernel and the well-known Favre Filtering is denoted as $\tilde{Q} := \overline{\rho Q}/\bar{\rho}$. On filtering Eq. (1) yields:

$$\frac{\partial \bar{\rho}\tilde{c}}{\partial t} + \nabla \cdot (\bar{\rho}\tilde{\boldsymbol{u}}\tilde{c}) + \nabla \cdot (\overline{\rho \boldsymbol{u} c} - \bar{\rho}\tilde{\boldsymbol{u}}\tilde{c}) = \overline{\nabla \cdot (\rho D \nabla c) + \dot{\omega}_c} \tag{2}$$

Here the turbulent LES sub-grid scale (sgs) scalar flux is denoted as $h_i = \overline{\rho u_i c} - \bar{\rho}\tilde{u}_i\tilde{c}$ where u_i is the ith component of velocity. Traditionally h_i is modelled using a gradient hypothesis,

$$h_i = -\frac{\mu_t}{Sc_t}\frac{\partial \tilde{c}}{\partial x_i} \tag{3}$$

with the eddy viscosity μ_t and the turbulent Schmidt number Sc_t, relying on the analogy of kinetic theory of gases. The above model mimics the greater extent of mixing in a turbulent flow by replacing the molecular diffusivity with an effective turbulent diffusivity and in addition has the desirable property of numerical stabilization. It always assumes a transport from regions with high values of $\tilde{c}$ to regions with low values of $\tilde{c}$. This type of model cannot account for situations where the turbulent flux is in the opposite direction, commonly called counter-gradient transport (CGT), occurring for example in geophysics and astrophysics (Starr 1968) or more general in

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complex two and three-dimensional flows (Younis et al. 2005, Rossi et al. 2010). Further, it is known for a long time (e.g. Tavoularis and Corrsin 1981) that even in flow configurations as simple as a statistically two-dimensional turbulent shear flow this assumption is wrong and Batchelor (1949) proposed a generalization by involving a turbulent diffusivity tensor instead of an isotropic value. The gradient transport approximation requires length and time scales of turbulence to be small in comparison with the corresponding mean flow scales and its application to radically different flows such as premixed turbulent flames is highly questionable (Libby and Bray 1981). Indeed it can be shown (Libby and Bray 1981) 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

$$h_i = \bar{\rho}\tilde{c}(1-\tilde{c})\left[\overline{(u_i)_P} - \overline{(u_i)_R}\right] \tag{4}$$

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 lower 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 $h_i > 0$. This result cannot be predicted by the gradient hypothesis (i.e. Eq. 3). The possibility of countergradient scalar transport in premixed turbulent flames was first hypothesized by Clavin and Williams (1979). A number of analyses demonstrated that counter-gradient transport can indeed be observed in the context of Reynolds Averaged Navier Stokes (RANS) simulations of turbulent premixed flames based on analytical (e.g. Bray et al. 1985; Mura and Champion, 2009), experimental (e.g. Moss, 1980; Cheng and Shepherd 1991; Frank et al. 1999; Kalt et al. 2002; Troiani et al. 2009) and computational (e.g. Rutland and Cant, 1994; Veynante et al. 1997; Swaminathan et al. 2001; Nishiki et al. 2006; Chakraborty and Cant, 2009a) analyses. A number of analyses (e.g. Veynante et al. 1997; Zimont and Biagioli, 2002; Nishiki et al. 2006; Chakraborty and Cant, 2009b; Sabelnikov and Lipatnikov, 2013) concentrated on RANS based closures of turbulent scalar flux. In the context of LES of premixed flames, turbulent scalar flux modelling has been investigated for example by Boger et al., (1998), Weller et al., (1998), Rymer (2001), Tullis and Cant (2003), Richard et al., (2007), Pfadler et al., (2009), Lecocq et al., (2010). It has recently been demonstrated by Gao et al. (2015a, 2015b) by performing an a-priori analysis of turbulent premixed planar flames, that the models, which account for the alignment of local resolved velocity and scalar gradients, perform relatively better than other existing models, despite the fact that these models were originally developed for non-reactive flows. In fact it can be shown (Sagaut 1998) that these models implicitly rely on a scale similarity assumption. Using a scaling analysis as demonstrated later in this document, it can be seen that a link can be established between these scale similarity type models and Eq. (4) which was derived using the Bray-Moss-Libby (1985) analysis. Therefore this class of models provides an interesting alternative to existing scalar flux models commonly used for reactive flow simulations. Scale similarity models are known not to provide enough dissipation in an actual LES (Vreman et al. 1997). Recently Anderson and Domaradzki (2012) identified the sources of deficiency of the scale similarity models and suggested a new model for momentum transport in the context of LES of incompressible flows. The purpose of this paper is:

- To discuss scale similarity type sub-grid scalar flux models in premixed turbulent combustion, which is rarely done in literature.
- To adapt the interscale energy transfer model for scalar transport in compressible reacting flows and to compare it to other scale similarity type models as well as a representative number of traditional models used in the literature for the closure of sub-grid scalar flux in premixed flames.
- To extend the earlier correlation analyses at the vector level (Gao et al. 2015a, 2015b) to the correlation analysis at the scalar level.
- To study the influence of density weighting (i.e. $\bar{\rho}(\widetilde{\tilde{u}_i\tilde{c}} - \tilde{\tilde{u}}_i\tilde{\tilde{c}})$ versus $\overline{\bar{\rho}\tilde{u}_i\tilde{c}} - \overline{\bar{\rho}\tilde{u}_i}\ \overline{\bar{\rho}\tilde{c}}\ /\ \overline{\bar{\rho}}$ see Eqs. (14) and (17)) on the performance of scale similarity type models in the context of turbulent premixed combustion.
- To extend Clark's tensor diffusivity by including higher order terms and demonstrate the new models performance.

2. DNS database

Two simple chemistry DNS databases of turbulent premixed flames have been considered for the current analysis. The physical mechanisms responsible for gradient/counter gradient transport are dependent on the competition between the turbulent velocity fluctuation and the velocity jump across the flame brush due to heat release. Thus, at the least, the qualitative behaviour of SGS scalar flux will not be different even if one uses complex instead of single step chemistry. The first database consists of five flames (i.e. cases A1-E1) with global Lewis number $Le = 0.34$, 0.6, 0.8, 1.0 and 1.2. In the presence of several different species, it is often difficult to assign a global Le and the Lewis number of deficient species is often taken to be the characteristic Le (Mizomoto et al., 1984). The effective Lewis number for a homogeneous fuel-air mixture was evaluated by Law and Kwon (2005) based on the heat release rate, whereas Dinkelacker et al., (2011) proposed a methodology of estimating effective Lewis number based on linear combination of fuel diffusivities in terms of their mole fractions. The unity Lewis number flame represents the stoichiometric methane-air flame, whereas the $Le = 0.34$ case is representative of a lean hydrogen-air mixture. The Lewis number 0.6 and 0.8 cases are representative of hydrogen-blended methane-air mixtures (e.g. 20 and 10% (by volume) hydrogen blended methane-air flames with overall equivalence ratio of 0.6) and the Lewis number 1.2 case is representative of a hydrocarbon-air mixture involving a hydrocarbon fuel which is heavier than methane (e.g. ethylene-air mixture with equivalence ratio of 0.7) (Kobayashi et al., 1996; Law and Kwon, 2004; Muppala et al., 2005; Dinkelacker et al., 2011).

The second database consist of five freely propagating statistically planar turbulent premixed flames (i.e. cases A2-E2) with a range of different $Re_t = 22,\ 23.5,\ 49,\ 100,\ 110$ where the values of Re_t were chosen to vary by changing Ka (Da) while keeping Da (Ka) unaltered. Moreover, u'/S_L increases from case A2 to E2.

The Lewis number, the initial values of normalised turbulent root-mean-square (rms) velocity fluctuation u'/S_L, integral length scale to thermal flame thickness ratio 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 listed in Tables 1 and 2, where S_L is the unstrained laminar burning velocity, $\delta_{th} = (T_{ad} - T_0)/\max|\nabla T|_L$ is the thermal flame thickness with T, T_{ad} and T_0 being the dimensional temperature, adiabatic flame temperature and the reactant temperature respectively. Note that the subscript 'L' refers to the unstrained laminar flame quantities. The heat release parameter $\tau = (T_{ad} - T_0)/T_0$ and the Zel'dovich number $\beta = T_{ac}(T_{ad} - T_0)/T_{ad}^2$ are taken to be 4.5 and 6.0 respectively where T_{ac} is the activation temperature. Standard values of Prandtl number ($Pr = 0.7$) and ratio of specific heats ($\gamma_g = 1.4$) have been used. For the Lewis (Reynolds) number database the simulation domain is taken to be a cube of $24.1\ \delta_{th} \times 24.1\ \delta_{th} \times 24.1\ \delta_{th}$

Table 1
Initial values of simulation parameters and non-dimensional numbers for the Lewis number DNS database.

Cases	Le	u'/S_L	l/δ_{th}	τ	Da	Ka
A1	0.34	7.5	2.45	4.5	0.33	13.0
B1	0.6	7.5	2.45	4.5	0.33	13.0
C1	0.8	7.5	2.45	4.5	0.33	13.0
D1	1.0	7.5	2.45	4.5	0.33	13.0
E1	1.2	7.5	2.45	4.5	0.33	13.0