A-priori Direct Numerical Simulation assessment of sub-grid scale stress tensor closures for turbulent premixed combustion

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Abstract
It is well-known that the flame normal acceleration due to chemical heat release significantly affects turbulent flow statistics within flames but limited effort has been directed to the assessment of sub-grid scale (SGS) stress tensor closures in turbulent premixed combustion. In the present analysis the closures of 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 turbulent Reynolds numbers. A family 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 (Phys. Fluids, vol. 24, 065104, 2012) has been extended for application to compressible flows and included in the analysis. Detailed physical explanations have been provided for the observed model performances.

Introduction

Turbulent combustion modeling 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, i^{th} 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 modeled 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. 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:

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

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 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 $F_i^{sgs} > 0$. This result cannot be predicted from classical gradient hypothesis closure. An expression for the SGS stress tensor may be obtained in the following manner subject to assumption of the presumed bi-modal sub-grid PDF of c with impulses at $c = 0$ and 1.0 [3,4]:

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

where $[\overline{(u_i u_j)}_R - \overline{(u_i)_R}\ \overline{(u_i)_R}]$ and $[\overline{(u_i u_j)}_P - \overline{(u_i)_P}\ \overline{(u_i)_P}]$ are the conditionally filtered SGS stresses in products and reactants respectively. Thus the magnitude and the sign of the stress depend on the relative magnitudes of the conditional velocities and on the conditional SGS stresses $[\overline{(u_i u_j)}_R - \overline{(u_i)_R}\ \overline{(u_i)_R}]$

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and $[\overline{(u_i\, u_j)}_P - \overline{(u_i\,)}_P\ \overline{(u_i\,)}_P]$. Thus it is unlikely that the commonly used Smagorinsky model, relying on the Boussinesq assumption, will be able to satisfactorily predict the SGS stresses in turbulent premixed flames. Indeed Pfadler *et al.* [2] demonstrated its weak performance based on direct measurements of the density weighted stress tensor. Although several publications deal with the modeling 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.

DNS database

In the present analysis the closures of SGS stress tensor have been *a-priori* assessed with respect to explicitly filtered Direct Numerical Simulation (DNS) data of freely propagating statistically planar turbulent premixed flames. The DNS database, described in detail in Ref. [7], has been explicitly filtered using a Gaussian filter kernel using seven different filter width 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 normalized root mean square turbulent velocity fluctuation u'/S_L, the ratio of turbulent integral length scale to flame thickness l/δ_{th} , Damköhler number $Da = lS_L/\delta_{th}u'$, Karlovitz number and turbulent Reynolds number $Ka = (u'/S_L)^{3/2}(l/\delta_{th})^{-1/2}$ and $Re_t = \rho_0\, u'l/\mu_0$ are provided in Table 1 where ρ_0 and μ_0 are the unburned gas density and viscosity respectively, $\delta_{th} = (T_{ad} - T_0)/Max\,|\nabla\hat{T}|_L$ 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. 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
Re_t	22.0	23.5	49.0	100	110
Da	0.33	0.23	0.33	0.48	0.33
Ka	8.65	13.0	13.0	13.0	19.5

Table 1 indicates that the cases A, C and E (B, C and D) have same values of Da (Ka) and Ka (Da) is modified to bring about the changes in Re_t. 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. All the simulations have been carried out for one chemical time scale (i.e. $t = \delta_{th}/S_L$).

Instantaneous views of isosurfaces for cases A 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. Further details are omitted for the sake of brevity and the reader is referred to Ref. [7] for additional information. For the sake of brevity, results will mostly be shown for cases A and E. The cases B, C, D follow the trends demonstrated by cases A and E.

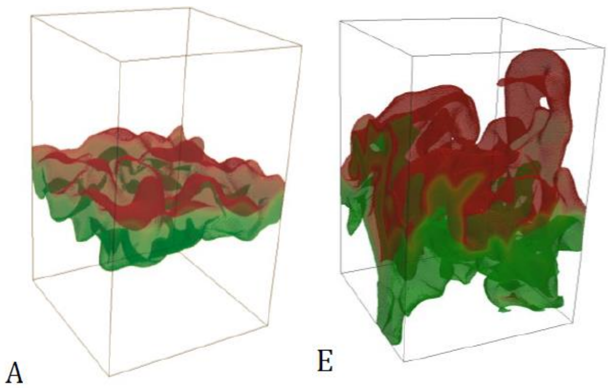

Figure 1. Instantaneous view of c isosurfaces for cases A and E at $t = \delta_{th}/S_L$. The value of c increases from 0.01 to 0.99 from green to red.

Sub-grid scale stress closure

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 [8]. 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 than given by the expression:

$$\tau_{ij}^{SSM} = -\bar{\rho}\nu_t 2\left(\widetilde{S_{ij}} - \frac{1}{3}\,\widetilde{S_{kk}}\delta_{ij}\right)$$
$$\nu_t = (C_s\Delta)^2\sqrt{2\,\widetilde{S_{ij}}\widetilde{S_{ij}}},\ \ \widetilde{S_{ij}} = \frac{1}{2}\left(\frac{\partial\widetilde{u_i}}{\partial x_j} + \frac{\partial\widetilde{u_j}}{\partial x_i}\right) \tag{5}$$

The constant C_s is either set to $C_s \approx 0.18$ in the static model version (SSM) or determined in a dynamic manner (DSM), for details see e.g. Ref. [8]. If one considers a statistically planar flame propagating in negative x_1 direction one obtains, assuming $\partial\widetilde{u_2}/\partial x_2 = \partial\widetilde{u_3}/\partial x_3 = 0$ and $\partial\widetilde{u_1}/\partial x_1 > 0$ due to heat release: $\tau_{11}^{SSM} = -\bar{\rho}\nu_t\frac{4}{3}\widetilde{S_{11}} \sim -\partial\widetilde{u_1}/\partial x_1 < 0$, i.e. τ_{11}^{SSM} assumes a negative value. A comparison between this behaviour with the prediction of eq. (4) reveals strictly positive values of the component τ_{11}^{SGS} , which in turn indicates the need for more advanced SGS stress modelling. This is in agreement with the experimental observations of Pfadler *et al.* [2]. In Refs. [5,6] it is shown, based on numerical and theoretical arguments, that in the context of SGS scalar flux modelling for turbulent premixed flames Clark's gradient model [9], and henceforth denoted as the CGM model, is very successful in representing gradient (GT) as well as counter gradient transport (CGT). Thus, this model is also considered in this analysis. The CGM model is given as:

$$\tau_{ij}^{CGM} = \bar{\rho}\frac{\Delta^2}{12}\frac{\partial \tilde{u}_i}{\partial x_k}\frac{\partial \tilde{u}_j}{\partial x_k} \qquad (6)$$

Closely related to the CGM is the so called scale similarity model [8], denoted as the VSS model in the following because the scale similarity hypothesis acts on the velocity components.

$$\tau_{ij}^{VSS} = \bar{\rho}\left(\overline{\tilde{u}_i\tilde{u}_j} - \bar{\tilde{u}}_i\,\bar{\tilde{u}}_j\right) \qquad (7)$$

Still another scale similarity model can be defined in the context of Favre filtering following Vreman [10]:

$$\tau_{ij}^{DSS} = \overline{\bar{\rho}\tilde{u}_i\tilde{u}_j} - \overline{\bar{\rho}\tilde{u}_i}\,\overline{\bar{\rho}\tilde{u}_j}\,/\,\bar{\bar{\rho}} \qquad (8)$$

It will henceforth be referred to as the DSS model, i.e. density based scale similarity model, because the scale similarity assumption acts on ρu_i rather than u_i. Scale similarity models are known not to provide enough dissipation in an actual LES [10]. Recently Anderson and Domaradzki [11] 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. This model is only Galilei invariant under the assumption of incompressible flow. Therefore the following modification of this model is suggested which is Galilei invariant and symmetric:

$$\tau_{ij}^{IET} = \bar{\rho}\left(\widehat{\hat{\tilde{u}}_i\tilde{u}_j} + \widehat{\tilde{u}_i\hat{\tilde{u}}_j} - \hat{\tilde{u}}_i\hat{\tilde{u}}_j - \widehat{\hat{\tilde{u}}_i\hat{\tilde{u}}_j}\right) \qquad (9)$$

It will henceforth be denoted as the IET model, i.e. interscale energy transfer model. Whenever a secondary filtering operation is required, throughout this work, the filter suggested by Anderson and Domaradzki [11] is used. The one dimensional filter coefficients are given by $(C, 1-2C, C)$ where the constant C is a free parameter with $0 < C \leq 1/3$. A typical value corresponds to $C = 1/12$. The three- dimensional filter is given by the convolution of three one dimensional filters of the above type.

Results and Discussion

According to the arguments put forward by Veynante *et al.* [12] in the context of SGS scalar flux one can expect a decreasing (increasing) extent of CGT (GT) with increasing u'/S_L. Hence, it is interesting to study the alignment of SGS stresses and the right hand side of eq. (5) in response to different turbulence intensities. However, the SGS stresses involve a tensor rather than a vector and hence the analysis is split into the SGS contributions to each individual component of the momentum transport (see eq. (2)). Figure 2 shows the cosine of the angle Θ between SGS stresses τ_{1j}^{SGS} evaluated from DNS and τ_{1j}^{SSM} for both extreme cases A and E and four different filter widths (note that the flame is propagating in negative x_1-direction). Since the Boussinesq hypothesis is a generalization of the gradient flux assumption the term GT (CGT) is used (somewhat imprecisely) in the following if the above defined angle Θ is 0^0 (180^0) and the cosine of the angle assumes the value 1.0 (-1.0).

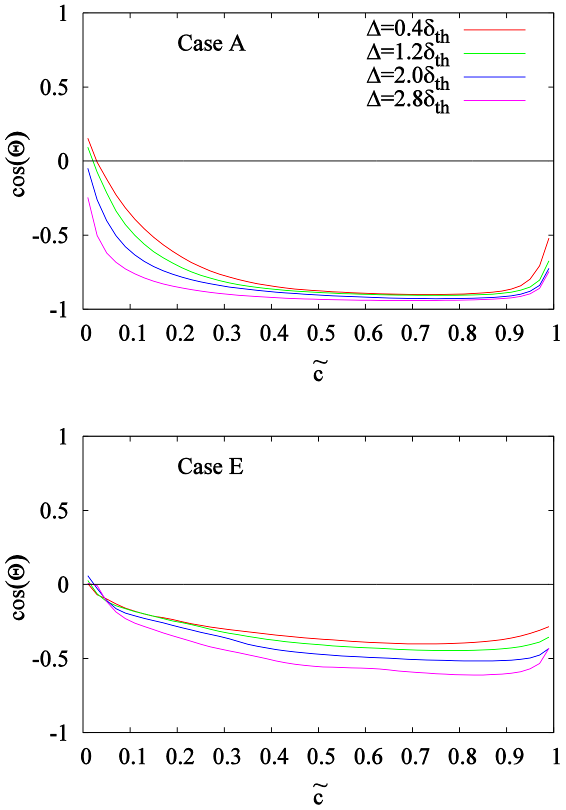

Figure 2. Cosine of the angle Θ between τ_{1j}^{SGS} calculated from DNS and τ_{1j}^{SSM} predictions conditional on $\tilde{c}$ for cases A and E, for four different filter width $\Delta \approx 0.4\delta_{th}, \Delta \approx 1.2\delta_{th}, \Delta \approx 2.0\delta_{th}, \Delta \approx 2.8\delta_{th}$.

Figure 2 shows that the extent of CGT increases with increasing filter width, which is similar to the behaviour observed for the SGS scalar flux [5,6]. Furthermore case A exhibits a higher extent of CGT than in case E because the effects of heat release are more likely to dominate over the effects of turbulent velocity fluctuation in case A than in case E. The behaviour is qualitatively similar to the one reported for SGS scalar flux in Refs. [5,6]. Since the x_2 and x_3 components are statistically identical only the x_2-component is discussed further in Fig. 3. The effects of heat release are less pronounced in the direction normal to the mean flame propagation. Consequently, the extent of CGT is smaller in Fig. 3 than in Fig. 2, which is consistent with earlier analysis [5,6]. However, contrary to Fig. 2 the amount of GT increases with increasing filter width. This can be explained by the fact that the term $\widetilde{S_{11}}$ in the isotropic part of eq. (5) dominates the model in x_2-direction. Figure 3 shows essentially the effect of an increasing amount of SGS dilatation with increasing filter width since the two minus signs cancel each other.

denominator and numerator of the C_s expression [8] separately in x_2 and $x_3$direction. No clipping is applied. Other averaging procedures (see Ref. [8]) gave qualitatively the same result (not shown here).

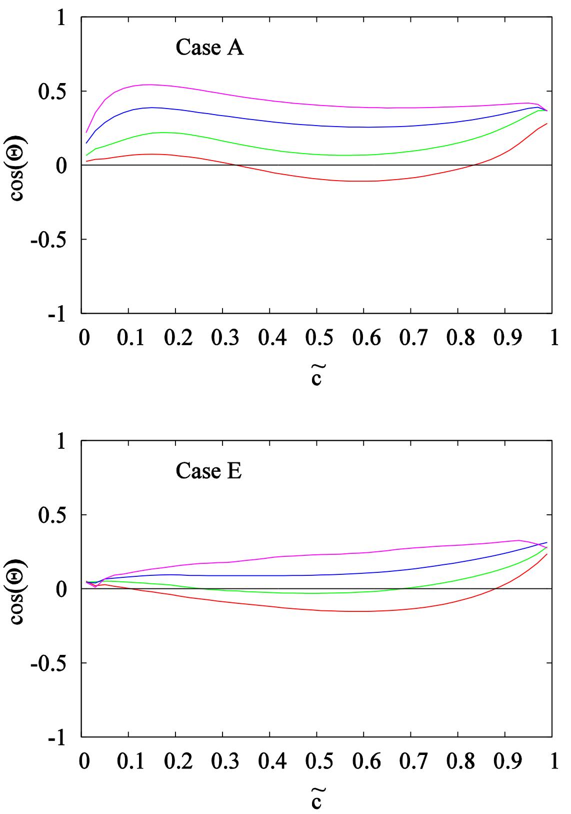

Figure 3. Cosine of the angle Θ between τ_{2j}^{SGS} calculated from DNS and τ_{2j}^{SSM} predictions conditional on $\tilde{c}$ for cases A and E, for four different filter width (legend same as in Fig. 2).

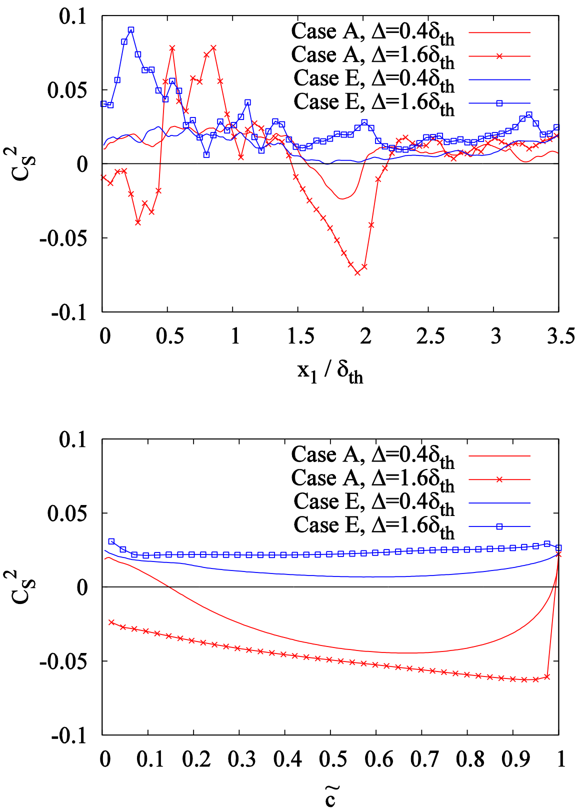

Figure 4. Variation of the Smagorinsky parameter C_s^2. In the upper part of the figure C_s^2 is determined after spatial averaging of numerator and denominator of the C_s^2 expression. In the lower part averages are calculated conditional on $\tilde{c}$.

Before analyzing the performance of the models given by equations (5)-(9) it is important to understand their sensitivity on the model parameters involved. All scale-similarity type models (eqs. (7)-(9)) depend on the width of the secondary filter which is in the framework of this investigation given by a parameter C. Preliminary investigations revealed for this particular database a weak dependence of the correlation coefficient on the secondary filter width and therefore $C = 1/12$ was used following the suggestion of Anderson and Domaradzki [11]. The Smagorinsky parameter C_s can be determined using a dynamic procedure as summarized for example in Ref. [8]. In more detail a model parameter is determined which corresponds to C_s^2, provided the parameter is positive. In order to avoid additional notation the expression C_s^2 is used here, even in case of a negative result. Typically, this constant needs a regularization, like averaging and clipping to ensure good numerical properties. Fig. 4 shows the Smagorinsky parameter for cases A and E, for a small and medium filter size. For larger filter size the result looks even noisier. In the upper part of the figure, the constant is calculated by averaging

In the lower part of the Fig. 4 conditional averaging (of the denominator and numerator) based on $\tilde{c}$ is applied in order to determine C_s^2. Figure 4 demonstrates that application of a standard averaging procedure for determining the parameter C_s^2 yields rather unsatisfactory results in the context of turbulent premixed combustion. The parameter fluctuates considerably in particular for high turbulence intensities and for large filter widths. As a result, the DSM model can perform even worse (not shown in this paper) than its static counterpart SSM. In contrast the lower part of the figure demonstrates clearly that the Smagorinsky parameter should be a function of $\tilde{c}$. It can be seen that on the unburned gas side C_s^2 is close to its theoretical value (i.e. 0.0324). However, in the middle of the flame brush, C_s^2 becomes smaller and for small turbulence intensities, when the effects of heat release are more pronounced, even negative in agreement with Fig. 2. The findings from Figs. 2-4 suggest that the Boussinesq approximation is not at all suitable in the context of turbulent premixed combustion. Indeed, the correlation analysis in the next paragraph shows a very low and sometimes even negative correlation coefficient for the SSM model. A dynamic evaluation of the model parameter, cannot change the alignment of the modelled stress tensor, and under the assumption, that negative effective viscosities should be avoided, it cannot improve the situation substantially. For this reason results for the DSM model will not be discussed further.

The following assessment of the models is based on a correlation analysis and on the magnitude of the model expressions conditional on $\tilde{c}$ in comparison to the value obtained from DNS.

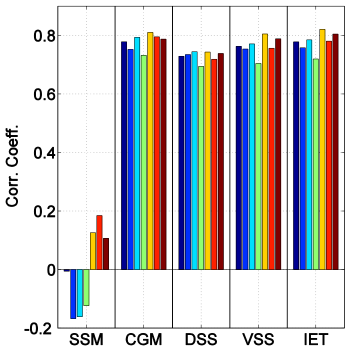

Figure 5. Correlation coefficients for the models SSM, CGM, DSS, VSS, IET for all the SGS stress components: τ_{mean} (■); τ_{11} (■); τ_{12} (■); τ_{13}(■); τ_{22} (■); τ_{23} (■) and τ_{33} (■). Results are averaged over all filter width and all cases.

Figure 5 shows the Pearson correlation coefficient for all models and all stress components τ_{ij} which are averaged over all filter width and all cases. In addition, τ_{mean} represents the mean value of all 6 components of τ_{ij}. It can be seen that the SSM model has low correlations with the SGS stress tensor. In particular, the predictions of the SSM model for all components involving contributions in the direction of mean flame propagation (i.e. τ_{1j}) are negatively correlated with DNS data. The remaining models which are all of scale similarity type show a similar correlation magnitude. The highest overall correlation coefficient is obtained for the CGM and the IET model. The differences in the DSS and VSS models are small.

Figures 6 and 7 show the variation of the conditional mean values of the different model predictions for the stress components τ_{11} and τ_{22} for cases A and E along with the corresponding DNS data for two different filter widths. The SSM model shows the unsatisfactory behavior prescribed already earlier. The CGM model performs very well for small filter width but underpredicts the stresses for large filter width. The VSS, DSS and IET models have similar mean values for small filter width but deviate more from each other for larger filter width. Overall their qualitative agreement with DNS data is reasonable. However, quantitatively no model is able to predict the stresses satisfactorily for all cases and all filter widths. The largest deviation occurs for Case A for large filter widths, where the effects of heat release dominate over the effects of turbulent velocity fluctuation. It will therefore be worthwhile to analyse the model behaviours for DNS data with different values of τ and *Le*.

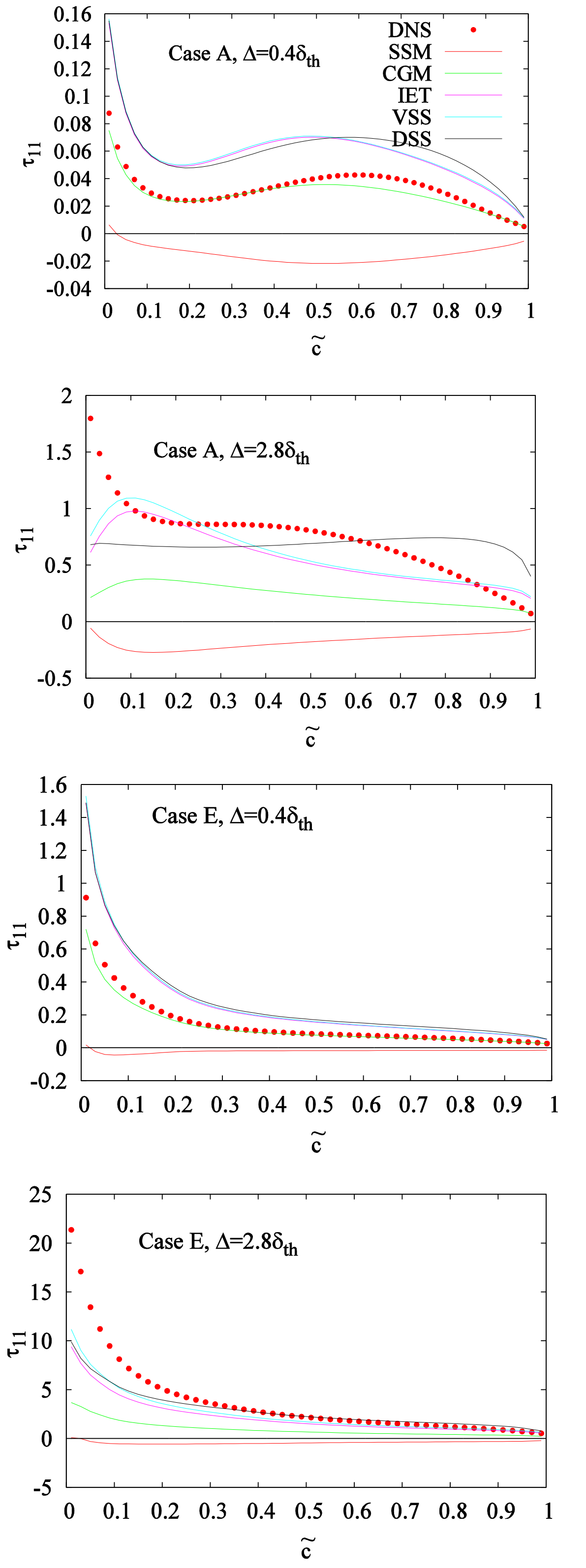

Figure 6. Conditional plot of τ_{11} calculated from DNS as well as different model expressions against $\tilde{c}$ for filter width $\Delta \approx 0.4\delta_{th}, \Delta \approx 2.8\delta_{th}$ for cases A and E.

Conclusions

The performance of several SGS stress models has been assessed in the context of LES of turbulent premixed flames based on *a-priori* analysis of DNS data for a range of different turbulent Reynolds numbers. The main focus was the evaluation of scale similarity type models, which showed a very promising behavior for scalar flux modelling. In addition to well-known models, a more recent development by Anderson and Domaradzki [11] is extended for application to compressible flows and included in the analysis. The results demonstrate that counter-gradient transport occurs not only for the scalar fluxes but also for the components of the SGS stress tensor that involve the component in the direction of mean flame propagation. Therefore the SSM and DSM models have a very low correlation coefficient. It is shown that the dynamic evaluation of the model parameter in the DSM model can be substantially improved if averaging conditional on the reaction progress variable is used. Nevertheless the underlying Boussinesq assumption remains invalid. The scale similarity type models investigated in this work show promising results. However, a more detailed investigation is needed to distinguish better between the different variants of these models. Of particular importance is the assessment of the dissipation characteristic of the different models which should ideally be assessed based on a-posteriori analysis.

Acknowledgments

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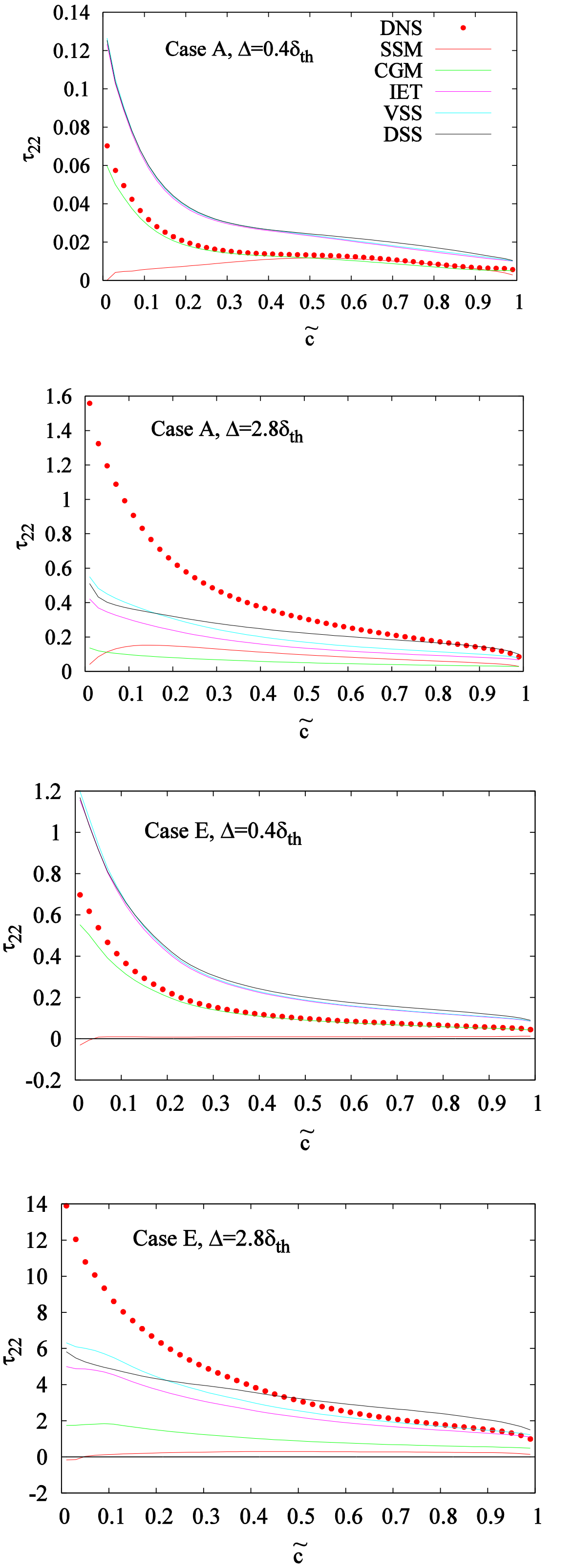

Figure 7. Conditional plot of τ_{22} calculated from DNS as well as different model expressions against $\tilde{c}$ for filter width $\Delta \approx 0.4\delta_{th}, \Delta \approx 2.8\delta_{th}$ for cases A and E.