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COMPARATIVE STUDY OF SUBFILTER SCALAR DISSIPATION RATE AND MIXTURE FRACTION VARIANCE MODELS

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Abstract. Accurate characterisation of mixing at the subfilter level is a critical aspect in many LES combustion models, such as flamelet based and Conditional Moment Closure models. Several models can be found in the literature, which vary from algebraic relations between resolved magnitudes, to the full transport of the subfilter magnitudes. In this paper a comparative between different published models is made in the context of a flamelet based combustion model. A turbulent hydrogen/methane flame is used as test case.

1 INTRODUCTION

The evaluation of the subgrid mixture fraction variance and the subfilter scalar dissipation rate is a critical issue in flamelet/flamelet progress-variable (FPV) models as well as Conditional Moment Closure (CMC) models. Both parameters model scalar mixing at the subgrid level, which in turn controls the combustion process. Therefore, accurate description of the subgrid mixing is critical as the Reynolds number is increased. The first proposed models to evaluate both quantities were based on a local equilibrium hypothesis, where production and destruction of variance at the subfilter level were assumed to cancel out. The proposed algebraic model [1], although being computationally efficient, was found to produce erroneous estimations of the scalar mixing in technically relevant flow configurations [2], thus being not suitable in many cases of industrial interest.

In the past several models have been proposed to account for deviations from local equilibrium, which model the subgrid mixture fraction variance and dissipation rate. One

option in order to take into account non-equilibrium effects is to construct a transport equation for the variance itself (VTE). Alternatively, being the variance an statistical quantity, it can be computed through its definition. The variance can be computed as $\widetilde{Z_v} = \widetilde{Z^2} - \widetilde{Z}^2$, which would in turn require computing the second moment of the mixture fraction, $\widetilde{Z^2}$. A transport equation for $\widetilde{Z^2}$ is then usually used (STE). However, in both cases closure for the subfilter dissipation rate is required. Algebraic expressions relating the subgrid variance with the subfilter dissipation through a turbulent time scale have been proposed [2, 3]. Additionally, closure for the scalar dissipation rate can also be performed through solving a transport equation it [4]. Each approach requires solving different equations and using different closures. Therefore, it is of interest to compare the behaviour of each model.

In the present study a large eddy simulation (LES) of a methane/hydrogen diffusion flame [5] using the flamelet/progress-variable model [6] is performed to study the behaviour of different models for the subfilter mixture fraction variance and subfilter scalar dissipation rate. The comparative shall put forth the strengths and weaknesses of each model.

2 MATHEMATICAL FORMULATION

Combustion models such as flamelet and CMC for turbulent diffusion flames usually use a passive scalar, the mixture fraction Z, which describes the mixing process. In LES, its transport equation takes the form

$$\frac{\partial \overline{\rho}\widetilde{Z}}{\partial t} + \frac{\partial \overline{\rho}\widetilde{u}\widetilde{Z}}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\overline{\rho}(\widetilde{D}_Z + D_{t,Z})\frac{\partial \widetilde{Z}}{\partial x_i}\right) \tag{1}$$

where $\overline{\rho}$ is the filtered density, and $\widetilde{Z}$ and $\widetilde{u}_i$ are the Favre filtered mixture fraction and velocity, respectively. Grid-based implicit filtering $\bar{\cdot}$, characterized by a filter length Δ, is related to Favre filtered quantities $\widetilde{\cdot}$ through $\widetilde{\phi} = \overline{\rho\phi}/\overline{\rho}$. Molecular diffusivity is represented by $\widetilde{D}_Z$ and turbulent subgrid scalar fluxes are modelled using an eddy-diffusivity assumption, being $D_{t,Z}$ the turbulent subgrid diffusivity. In order to comprehensively describe the combustion state, models for the subfilter mixing are required, namely the subfilter variance Z_v and the scalar dissipation rate $\widetilde{\chi}_Z$. In LES, the scalar variance, or second central moment, defined in terms of a probability density function (*pdf*) [7] is

$$Z_v = \widetilde{Z^2} - \widetilde{Z}^2 \tag{2}$$

where Z_v denotes the subfilter mixture fraction variance.

If production and destruction of the mixture fraction variance at the small scales is assumed to be in equilibrium [1, 8], the scalar dissipation rate becomes

$$\widetilde{\chi}_Z = 2(\widetilde{D}_Z + D_{t,Z})\frac{\partial \widetilde{Z}}{\partial x_i}\frac{\partial \widetilde{Z}}{\partial x_i} \tag{3}$$

With the local equilibrium assumption (LEA), the mixture fraction variance is computed through a scale similarity model [1]

$$\overline{\rho} Z_v = C_{var} \Delta^2 \overline{\rho} |\nabla \widetilde{Z}| \tag{4}$$

where C_{var} is calculated using the *Leonard term Expansion Dynamic model* (LED) [9]. Within the dynamic evaluation, in the model terms a top-hat test filter with filter size $\hat{\Delta} = 2\Delta$ is used.

If non-equilibrium effects are to be considered, Eq. (3) cannot be used, thus alternative closures for the subfilter dissipation rate have to be used. If the variance is computed through Eq. (2), then, $\widetilde{Z^2}$ is usually computed through a transport equation for the second moment of the mixture fraction (STE).

$$\frac{\partial \rho \widetilde{Z^2}}{\partial t} + \frac{\partial \overline{\rho} \widetilde{u} \widetilde{Z^2}}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\overline{\rho} (\widetilde{D_Z} + D_{t,Z}) \frac{\partial \widetilde{Z^2}}{\partial x_i} \right) - \overline{\rho} \widetilde{\chi}_Z \tag{5}$$

Otherwise, a variance transport equation (VTE) may be constructed

$$\frac{\partial \rho Z_v}{\partial t} + \frac{\partial \overline{\rho} \widetilde{u} Z_v}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\overline{\rho} (\widetilde{D}_Z + D_{t,Z}) \frac{\partial Z_v}{\partial x_i} \right) + 2 \overline{\rho} (\widetilde{D}_Z + D_{t,Z}) \frac{\partial \widetilde{Z}}{\partial x_i} \frac{\partial \widetilde{Z}}{\partial x_i} - \overline{\rho} \widetilde{\chi}_Z \tag{6}$$

$$\widetilde{\chi}_Z = 2 \widetilde{D}_Z \widetilde{\frac{\partial Z}{\partial x_i} \frac{\partial Z}{\partial x_i}} = 2 \widetilde{D}_Z \frac{\partial \widetilde{Z}}{\partial x_i} \frac{\partial \widetilde{Z}}{\partial x_i} + \chi_{Z,sgs} \tag{7}$$

where $\chi_{Z,sgs}$ is the subfilter dissipation rate.

Therefore, closure for the scalar dissipation rate, Eq. (7), is required in order to evaluate the subfilter mixture fraction variance. On the one hand, the subgrid variance can be related to the subfilter dissipation rate through a turbulent mixing timescale [2, 3]

$$\chi_{Z,sgs} = \frac{C_Z}{\tau} Z_v = C_Z \frac{\nu_t}{\Delta^2} Z_v \tag{8}$$

where τ is a turbulent mixing time scale, which is modelled through the turbulent viscosity ν_t. The model constant is of the form $C_Z = C_{\chi Z}(C_\varepsilon / C_u)$, where $C_{\chi Z} = 2$ is a constant relating mechanical and scalar time scales and $(C_\varepsilon / C_u) = 2$ are constants related to the energy spectra [3].

On the other hand, closure for the scalar dissipation rate $\widetilde{\chi}_Z$ can be achieved by constructing a transport equation for it (SDR-TE) [4]. Evaluation of the SDR-TE requires

modelling several unclosed terms and the evaluation of computationally expensive terms.

$$\begin{aligned}\frac{D}{Dt}\left(\overline{\rho}\widetilde{|\nabla Z|^2}\right) &= \frac{\partial}{\partial x_i}\left(\overline{\rho}(\widetilde{D_Z}+D_{t,Z})\frac{\partial\widetilde{|\nabla Z|^2}}{\partial x_i}\right)\\ &- 2\overline{\rho}\left(\frac{\partial\widetilde{u}_i}{\partial x_j}\frac{\partial\widetilde{Z}}{\partial x_i}\frac{\partial\widetilde{Z}}{\partial x_j}\right) - 2\overline{\rho}\widetilde{D}_Z\left(\frac{\partial^2\widetilde{Z}}{\partial x_i\partial x_j}\right)\\ &- \frac{2}{\overline{\rho}}\frac{\partial\overline{\rho}}{\partial x_i}\frac{\partial\widetilde{Z}}{\partial x_i}\left(\frac{\partial}{\partial x_j}\left(\overline{\rho}\widetilde{D}_Z\frac{\partial\widetilde{Z}}{\partial x_j}\right)\right)\\ &+ 2\frac{\partial\overline{\rho}\widetilde{D}_Z}{\partial x_i}\frac{\partial\widetilde{Z}}{\partial x_i}\left(\frac{\partial^2\widetilde{Z}}{\partial x_j^2}\right) + 2\frac{\partial\widetilde{Z}}{\partial x_i}\frac{\partial\widetilde{Z}}{\partial x_j}\left(\frac{\partial^2\overline{\rho}\widetilde{D}_Z}{\partial x_i\partial x_j}\right)\\ &+ C_{prd}\overline{\rho}\frac{32\nu_t}{\Delta^2}\left(\widetilde{|\nabla Z|^2} - |\nabla\widetilde{Z}|^2\right)\\ &- 12C_{var}\overline{\rho}\frac{\widetilde{D}_Z}{Z_v}\left(\widetilde{|\nabla Z|^2} - |\nabla\widetilde{Z}|^2\right)^2\end{aligned} \tag{9}$$

where $C_{prd} = 1$ is a model constant and C_{var} is dynamically evaluated using the LED model.

Regarding both STE and VTE approaches, it has been shown that the calculation of the variance through its definition, Eq. (2), leads to lower numerical errors [10]. However, numerical errors in the $\widetilde{Z^2}$ equation can lead to considerable repercussion in the computed variance as pointed out by [4].

3 NUMERICAL SIMULATION

Numerical computations are performed using the general purpose unstructured and parallel object-oriented CFD code TermoFluids [11]. Modelling of the turbulent fluxes is performed using standard eddy diffusivity models, where the turbulent viscosity is evaluated using the WALE model [12]. A dynamic procedure has been applied to compute both mixture fraction and progess-variable turbulent scalar-diffusivities, following the method of Moin [13], with the modification of Lilly [14]. In the dynamic procedure, top-hat test filters were constructed by vertex connectivity.

The steady flamelet/progress-variable model (SFPVM) [6] is used to model chemistry-turbulence interactions. Differential diffusion effects were considered when constructing the flamelet library. The progess-variable was defined as the sum of the mass fractions of CO, CO_2, H_2 and H_2O. Turbulent variables are described using a β-pdf for the statistical distribution of the mixture fraction and a δ-pdf has been assumed for the progress-variable. The state relation for any thermochemical variable is then

$$\widetilde{\phi} = \widetilde{F}(\widetilde{Z}, \widetilde{Z_v}, \widetilde{c}) \tag{10}$$

The case of study is the axisymmetric jet flame known as DLR Flame A [5, 15]. It consists of a $D = 8mm$ wide jet with a thinned rim at the exit. The inner jet is composed of 33.2% H_2, 22.1% CH_4, and 44.7% N_2 by volume and the outer jet is regular air with 20.1% O_2. The cold jet exit bulk velocity is fixed to $42.15m/s$ resulting in a Reynolds number of $15,200$. The jet was mounted concentrically to the coflow nozzle, which had a diameter of $140mm$ and provided air at $0.3m/s$. Both fuel and coflow air were at $300K$. The stoichiometric mixture fraction is $Z_{st} = 0.167$.

Regarding the mesh, numerical simulations have been performed on a structured mesh concentrated near the central jet with 95x645x32 control volumes in the radial, axial and azimuthal directions respectively. Mesh sizes were compared against the kolmogorov scale for this case, and ratios ranging between 10 and 20 were found in the regions of interest, thus ensuring that the analysis was performed in the inertial range.

Four closures are considered: i) the algebraic model, which uses Eq. (3) and (4), ii) the VTE model, in which the transport equation for the variance is solved, Eq. (6), and $\chi_{Z,sgs}$ is closed using Eq. (8), iii) the SDR-TE model, where the transport equation for $\widetilde{Z^2}$ is used, Eq. (5), the transport equation for the scalar dissipation rate serves as closure Eq. (9), and the variance is computed through its definition Eq. (2), iv) the STE model, where transport of the second moment of the mixture fraction is performed through Eq. (5), closure for $\chi_{Z,sgs}$ is mafe using Eq. (8) and Eq. (2) is employed to compute the variance.

4 DISCUSSION

Figure 1 and 2 show the averaged values for the mixture fraction variance, Z_v, and the subfilter scalar dissipation rate, $\chi_{Z,sgs}$, respectively. Comparing the results obtained using the different models, several aspects may be stressed. First, when computing the mixture fraction variance using its statistical definition Eq. (2), as in the STE and SDR-TE models and depicted in Figure 1c-1d, its maximum value is significatively higher than in the algebraic, Figure 1a, and VTE models, 1b. Notice, that the maximum value is found close to the inflow boundaries. This difference may be explained by the different means of computation used by each model. The LED algebraic models the variance locally by assuming a scale similarity and using the mixture fraction and its gradient. The dynamic evaluation of the coefficient may be affected by clipped filtering test filters due to the proximity of the boundaries. The VTE computes the variance through its transport equation, and fixing a zero variance at the boundaries. The low values observed may be attributed to insuficient production of variance by the model at the subfilter level. On the other hand, STE and SDR-TE models compute the variance as the difference between $\widetilde{Z^2}$ and the square of the mixture fraction $\widetilde{Z}$. Two sources of errors may affect this last computation. In the transport equation of $\widetilde{Z^2}$ there is a model for the subgrid scalar dissipation rate, $\chi_{Z,sgs}$, which could introduce numerical inaccuracies in the computed value. Additionally, in Eq. (2), the filtered mixture fraction is squared, thus numerical errors may be magnified, and therefore affect the precision. Nonetheless, it can be seen,

that overall the four models are active in the same domain regions, although with different intensities.

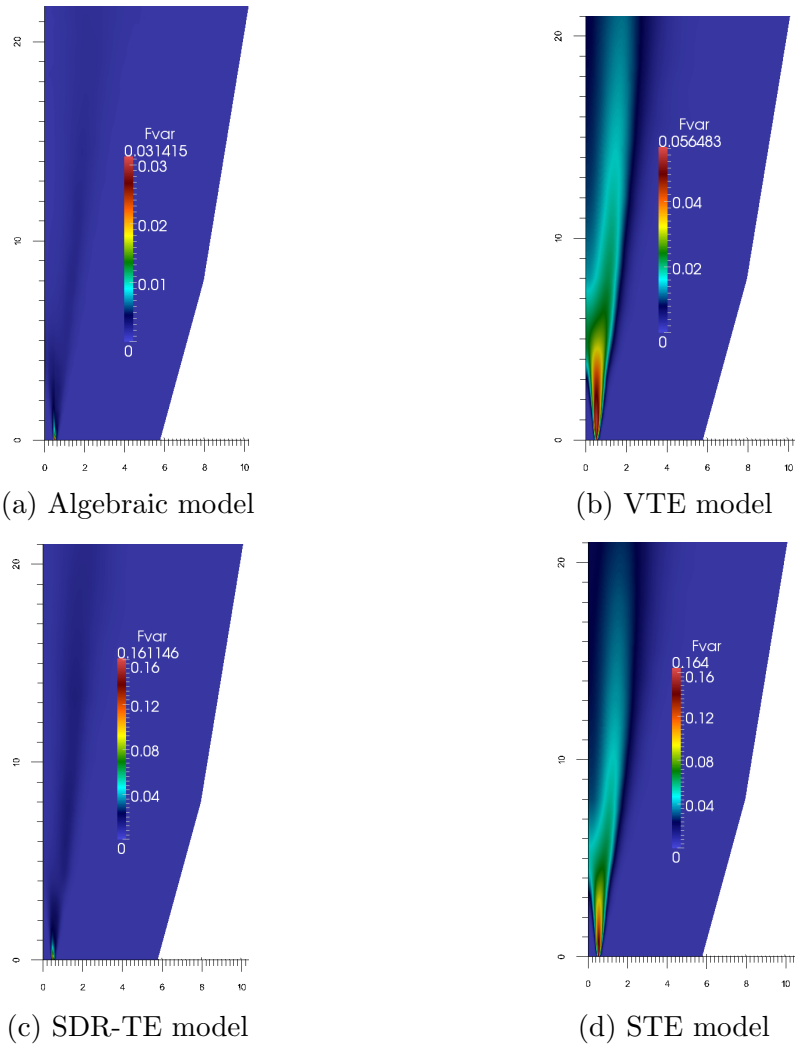
Then, if the domain layout of the mixture fraction is taken into account, it can be seen that the LED, Figure 1a, and the SDR-TE, Figure 1c, models predict a similar distribution, the maximum value is located close to the inflow boundaries and its value rapidly diminishes. In opposition, the VTE, Figure 1b, and STE, Figure 1d, predict a slower decrease of the mixture fraction variance value. This difference in behaviour may be explained by the differences seen in the distribution of $\chi_{Z,sgs}$. Both the LED algebraic model, Figure 2a, and SDR-TE, Figure 2c, give higher values for the subgrid scalar dissipation rate, whereas VTE and STE models produce lower values. Therefore, in can be seen that models which make direct use of gradients, as in the algebraic LED and the SDR-TE, produce sharper distributions of both quantities. Whereas, in the VTE and STE models, the subgrid scalar dissipation rate is computed from the mixture fraction variance using an algebraic relation, Eq. (8). A direct proportionality can be seen between the magnitude of the mixture fraction variance and the magnitude of the scalar dissipation rate for these models.

Taking into account the computed values, it has been shown by several authors that the algebraic model tends to underpredict the computed variance [4, 7, 10], which the results in Figure 1 confirm, as the variance computed using the algebraic model show the lowest values. Additionally, it has been argued that the VTE model underestimates the variance [10] compared to models using the transport equation for $\widetilde{Z^2}$, Eq. (5), either STE or SDR-TE models. As it can be seen from Figure 1, the VTE model Figure 1b presents lower values compared to STE based models, Figure 1d and 1c.

Regarding the computational costs, it must be stated that the algebraic model is the entails the lowest computational cost of the studied models, but at the cost of introducing strong assumptions in the computation. VTE and STE models were found to marginally increase the costs with respect to the algebraic model. The reason being that the computational cost of the dynamic procedure required for the algebraic model constant, Eq. (4), is similar to evaluating a transport equation. Finally, the SDR-TE model was the most expensive one, requiring twice the time of VTE or STE models to perform the same number of iterations.

5 CONCLUSIONS

Correct description of mixing at the subgrid level is critical to many LES combustion models. Several models have been presented in the literature to account for this subfilter mixing. Four representative models have been used in simulating a hydrogen-methane turbulent diffusion flame and their behaviour has been compared. The algebraic model [1, 9] has been shown to predict a smaller level of variance, which was in accordance to findings presented by other authors. Significant differences in the outcome of the VTE [3] and STE were found, although both models used the same closure for the subgrid



(a) Algebraic model

(b) VTE model

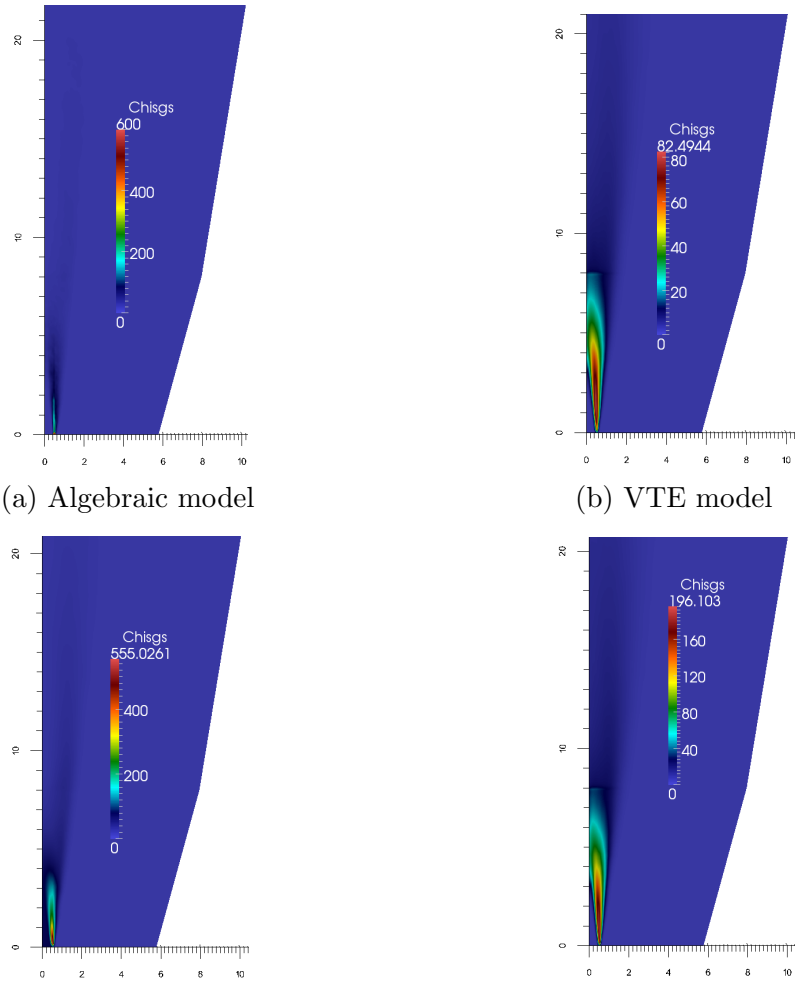
(c) SDR-TE model

(d) STE model

Figure 1: Subfilter mixture fraction variances, Z_v, computed with the different models. Axial and radial axes are plotted in non-dimensional form, using the jet diameter ($D = 8mm$) as reference value.

scalar dissipation rate, Eq. (8). Previously, it had been reported that the VTE model underpredicts the mixture fraction variance when compared to the transport of the second moment $\widetilde{Z^2}$ [10], and results here presented show a similar trend. Finally, the SDR-TE [4], has been found to predict high levels of subgrid scalar dissipation rate. Additionally, since the SDR-TE makes use of a transport equation for $\widetilde{Z^2}$, similar variance levels are obtained compared to the STE model.

From a computational point of view, both VTE and STE models have been found to efficiently incorporate non-equilibrium effects at a reasonable cost, compared to the algebraic model. The rationale behind it being that the dynamic evaluation of the algebraic



(a) Algebraic model

(b) VTE model

(c) SDR-TE transport model

(d) STE model

Figure 2: Subfilter scalar dissipation rate, $\chi_{Z,sgs}$, computed with the different models. Axial and radial axes are plotted in non-dimensional form, using the jet diameter ($D = 8mm$) as reference value.

model constant requires a filtering operation, which is computationally expensive. Transport of the scalar dissipation rate, SDR-TE, was found to be the most computationally expensive one.

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