A NON-EQUILIBRIUM MODEL FOR SCALAR DISSIPATION RATE IN LES OF COMBUSTION

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ABSTRACT

Modeling of subfilter scalar dissipation rate is critical to accurate simulation of turbulent combustion using large eddy simulation (LES). Non-equilibrium models contain a timescale coefficient $\mathscr{C}_\tau$ that is generally unknown a priori and cannot be determined by conventional dynamic modeling procedures. Here, an alternative dynamic procedure is formulated from the variance transport equation (VTE). The modeling accuracy of the VTE-based dynamic model for $\mathscr{C}_\tau$ is assessed through a priori tests in homogeneous isotropic turbulence and in a planar jet flow. Particular attention is given to the effects of various averaging methods used for coefficient estimation and a novel conditional averaging approach is presented.

INTRODUCTION AND MOTIVATION

The scalar dissipation rate is a fundamental parameter in the study of nonpremixed flames. In such flames, species mass fractions and temperature can be related to the mixture fraction Z, a conserved scalar (Bilger, 1980). Reactions are assumed to occur in a thin zone around iso-surfaces of the stoichiometric mixture fraction value. The scalar dissipation rate

$$\chi_Z = 2D\frac{\partial Z}{\partial x_i}\frac{\partial Z}{\partial x_i} \tag{1}$$

quantifies the rate at which small scale mixing occurs and is related to the relaxation time of the diffusive layer surrounding the reaction zone, with D denoting the scalar molecular diffusivity. This picture of flame structure is embodied by flamelet modeling, in which local thermochemistry is determined by the values of Z and χ_Z (Peters, 2000).

Large eddy simulation (LES) has become the preferred methodology for the simulation of nonpremixed turbulent combustion because it accurately predicts the mixing of fuel and oxidizer at large scales by solving for the filtered mixture fraction. Favre, or density-weighted, filtering is often used in variable density flows (Pitsch, 2006). The Favre filtered mixture fraction is defined as $\widetilde{Z} = \overline{\rho Z}/\bar{\rho}$, where $\overline{(\cdot)}$ indicates a spatial filtering operation at filterwidth Δ.

The molecular mixing characterized by χ_Z is associated with flow length scales far smaller than those present in the filtered scalar field. As a consequence, the filtered scalar dissipation $\widetilde{\chi_Z}$ is dominated by its unclosed subfilter component

$$\widetilde{\varepsilon_Z} = \widetilde{\chi_Z} - 2D\frac{\partial \widetilde{Z}}{\partial x_i}\frac{\partial \widetilde{Z}}{\partial x_i} \tag{2}$$

Since the second term in Eq. 2 can be computed directly from the LES filtered scalar solution, a model for either $\widetilde{\varepsilon_Z}$ or $\widetilde{\chi}_Z$ provides closure for both quantities. Here, models will be written for $\widetilde{\varepsilon_Z}$. Diffusivity is both a function of species composition and local temperature. In this work, this molecular diffusivity is denoted by D. It is assumed that all the species have equal diffusivity.

The subfilter scalar dissipation rate also appears in the transport equation for the subfilter mixture fraction variance, $Z_v = \widetilde{ZZ} - \widetilde{Z}\widetilde{Z}$, another key quantity in LES combustion modeling that characterizes the small scale fluctuations of Z. After closing subfilter flux terms using an eddy diffusivity D_T, the variance transport equation (VTE) is given by

$$\frac{\partial \bar{\rho} Z_v}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_i Z_v}{\partial x_i} = \frac{\partial}{\partial x_i}\left[\bar{\rho}\left(D + D_T\right)\frac{\partial Z_v}{\partial x_i}\right] + 2\bar{\rho} D_T \frac{\partial \tilde{Z}}{\partial x_i}\frac{\partial \tilde{Z}}{\partial x_i} - \bar{\rho}\widetilde{\varepsilon_Z} \tag{3}$$

Commonly, both the scalar variance and scalar dissipation rate are modeled by algebraic closures that assume a local equilibrium between variance production at resolved scales (modeled by the second term on the right hand side of Eq. 3) and dissipation at subfilter scales. This results in the model

$$\widetilde{\varepsilon_Z} = 2D_T \frac{\partial \widetilde{Z}}{\partial x_i} \frac{\partial \widetilde{Z}}{\partial x_i} \tag{4}$$

Girimaji and Zhou (1996) arrived at the same model by applying arguments from renormalization group theory.

However, variance can be predicted more accurately by using its modeled transport equation rather than an algebraic model (Kaul and Raman, 2011; Jimenez et al., 2001). Eq. 4 is unsuitable for use with the variance transport equation since the final equation form would contain no source or sink terms, erroneously causing variance to be conserved in a closed system (Jimenez et al., 2001). Instead, a common model (Peters, 2000) from Reynolds averaged simulations (RAS) is adapted to the LES context. This model can be written as

$$\widetilde{\varepsilon_Z} = \mathscr{C}_\tau \frac{Z_v}{\tau_Z} \tag{5}$$

where $\mathscr{C}_\tau$ is a model coefficient and τ_Z is a mixing timescale, given by expressions such as (Colucci et al., 1998; Jaberi et al., 1999; Raman and Pitsch, 2006)

$$\tau_Z = \frac{\Delta^2}{D + D_T} \tag{6}$$

As for any model in LES, Eq. 5 imperfectly captures the characteristics of the quantity it represents. A model of this type implicitly links production and dissipation by relying on a mixing timescale formed from filter scale variables and effectively assumes an energy cascade process (Fox, 2003; Pitsch, 2006). Despite the model's deficiencies, the fact remains that no alternative non-equilibrium model exists. Furthermore, from a practical standpoint, the most significant problem posed by the use of Eq. 5 is the determination of the model coefficient $\mathscr{C}_\tau$. The optimal value of this model coefficient is usually unknown a priori and depends on the flow under consideration and the chosen timescale expression. Furthermore, it must be recalled that in LES, unlike in RAS, $\mathscr{C}_\tau$ is a spatially and temporally varying quantity.

Dynamic procedures based on inertial range scaling arguments are often used to specify model coefficients in LES. These approaches infer the value of a subfilter scale quantity using information from the smallest filtered scales that is extracted by test filtering at a larger filterwidth $\widehat{\Delta}$. Dynamic procedures for estimating $\mathscr{C}_\tau$ have been put forth (Pera et al., 2006; Chumakov and Rutland, 2004). However, dissipation is a predominantly small scale quantity that cannot be reliably predicted from its content in an inertial range test window. Indeed, Pierce and Moin (1998) specifically avoided such a dynamic scalar dissipation model when proposing their dynamic variance model. Another dynamic estimation scheme is based on a global equilibrium assumption (Balarac et al., 2008) and predicts a single time-varying value of $\mathscr{C}_\tau$ for the entire flow domain. The total subfilter variance in a periodic flow domain remains constant under this model, although mixing should reduce subfilter variance with time.

Here, we present an alternative dynamic formulation in which $\mathscr{C}_\tau$ is calibrated from the rate of scalar energy transfer between test and filter scales, which can be estimated using the VTE. A similar approach has been used to develop a model for the viscous dissipation rate of the subfilter turbulent kinetic energy (Ghosal et al.,1995). However, the extreme importance of $\widetilde{\chi_Z}$ in combustion modeling should be recalled in addition to the function of $\widetilde{\varepsilon_Z}$ as a sink term for scalar variance. The dual role of the scalar dissipation rate makes its modeling a unique challenge.

Manipulation of the VTE, as described below, leads to a spatially localized expression for the model coefficient. The derivation of this expression is only the first step in the model's development. Model implementation raises further issues that will be investigated by applying a priori analysis methods to data from direct numerical simulation (DNS) of homogeneous isotropic turbulence and of a planar jet. Selection of an averaging procedure for evaluation of the model coefficient is one such aspect of model implementation that will be investigated here.

MODEL DERIVATION

The derivation of the dynamic scalar dissipation rate model is based on the idea that the variance transport equation can be applied at any filter scale falling within the inertial range. On a physical level the model can be understood in terms of a mixing cascade. It should be recalled that the assumption of a mixing cascade is already implicit in the formulation of Eq. 5. The dynamic procedure merely makes this assumption explicit. Eq. 3 is the VTE is written at the LES filter scale Δ. An analogous equation can be written at a test filter scale $\widehat{\Delta}$, with spatial filtering operation denoted by $\widehat{(\cdot)}$ and Favre filtering operation $\breve{(\cdot)}$, as

$$\frac{\partial \hat{\bar{\rho}} Z_t}{\partial t} + \frac{\partial \hat{\bar{\rho}} \breve{u}_i Z_t}{\partial x_i} = \frac{\partial}{\partial x_i}\left[\hat{\bar{\rho}}\left(D + D_T^t\right)\frac{\partial Z_t}{\partial x_i}\right] + 2\hat{\bar{\rho}} D_T^t \frac{\partial \breve{Z}}{\partial x_i}\frac{\partial \breve{Z}}{\partial x_i} - \mathscr{C}_\tau \hat{\bar{\rho}} \frac{Z_t}{\tau_Z^t} \tag{7}$$

In Eq. 7, Z_t is the sub-test filter variance, $Z_t = \breve{\widetilde{ZZ}} - \breve{Z}\breve{Z}$. A superscript t indicates a model quantity evaluated at the test filter level, e.g. D_T^t. The test filterwidth is typically taken to be twice the LES filterwidth, $\widehat{\Delta} = 2\Delta$. Test filtering Eq. 3 and subtracting it from Eq. 7 gives the relationship

$$\mathscr{C}_\tau X = Y = F + P - T \tag{8}$$

if it is assumed that $\mathscr{C}_\tau$ varies slowly in space and can be removed from the test filtering operation applied to Eq. 3. The quantity X on the left hand side of Eq. 8 is given by

$$X = \hat{\bar{\rho}} \frac{Z_t}{\tau_Z^t} - \widehat{\left(\bar{\rho}\frac{Z_v}{\tau_Z}\right)} \tag{9}$$

The first two terms on the right hand side of Eq. 8 represent the differences in convective and diffusive fluxes

$$F = \frac{\partial}{\partial x_i}\left[\widehat{\bar{\rho}\tilde{u}_i Z_v} - \bar{\rho}\widehat{(D+D_T)\frac{\partial Z_v}{\partial x_i}} - \hat{\bar{\rho}}\check{u}_i Z_t + \hat{\bar{\rho}}(D+D_T^t)\frac{\partial Z_t}{\partial x_i}\right] \tag{10}$$

and in production

$$P = 2\hat{\bar{\rho}} D_T^t \frac{\partial \check{\tilde{Z}}}{\partial x_i}\frac{\partial \check{\tilde{Z}}}{\partial x_i} - 2\widehat{\bar{\rho} D_T \frac{\partial \tilde{Z}}{\partial x_i}\frac{\partial \tilde{Z}}{\partial x_i}} \tag{11}$$

of variance at the test and filter scale. The third term represents accumulation or loss of scalar energy between filter and test scales

$$T = \frac{\partial \hat{\bar{\rho}} L_v}{\partial t} \tag{12}$$

where L_v is the variance Leonard term given by

$$L_v = \widecheck{\tilde{Z}\tilde{Z}} - \check{\tilde{Z}}\check{\tilde{Z}} \tag{13}$$

Note that $L_v = Z_t - \check{Z}_v$. Since L_v can be computed directly from the resolved scalar fields, this relationship can be used to compute Z_t from the the known values of Z_v and $\widetilde{Z}$.

The grouping of terms used here was chosen to highlight their phenomenological characteristics. However, other orderings may be more efficient from a computational standpoint, for example to reduce the number of test filtering operations required. It should be recognized that many of the quantities in the model are terms from the filter level VTE that can be reused by the dynamic procedure. Similarly, the test filter level eddy diffusivity, D_T^t can be computed with minimal additional cost. If, at the LES filter level, $D_T = \mathscr{C}_Z \Delta^2 |\tilde{S}|$ is modeled dynamically (Moin et al.,1991) by assuming the model coefficient $\mathscr{C}_Z$ is scale invariant, it is then consistent with that assumption to use $D_T^t = \mathscr{C}_Z \widehat{\Delta}^2 |\check{S}|$, $\mathscr{C}_Z$ having the same value in both expressions. The magnitude of the strain rate tensor at the test filter level is already required by the dynamic eddy diffusivity modeling procedure.

AVERAGING APPROACHES FOR MODEL IMPLEMENTATION

Although Eq. 8 encapsulates the basic dynamic dissipation rate modeling idea, additional factors must be considered to put the model to use in simulations. Choices made in model implementation can significantly affect predicted coefficient values. Here we consider various averaging approaches that can be employed for coefficient prediction.

The model is evaluated through a priori tests on data from DNS of two different flows. The first is homogeneous isotropic turbulence (HIT), simulated using pseudospectral methods on a 512^3 periodic domain. The velocity field was forced to maintain $\mathrm{Re}_\lambda = 135$ while the scalar field was decaying. Results are shown for a filterwidth $\Delta = 16\eta$, where η is the Kolmogorov length. The second configuration is a piloted planar jet with Reynolds number (based on jet width H and average jet-to-coflow velocity difference) of 6000. The computational domain extends $20H$ in the streamwise direction x, $15H$ in the stream-normal direction y, and $2.56H$ in the periodic spanwise direction z. It is discretized by $768 \times 512 \times 128$ in the x, y, and z directions, respectively.

Germano Averaging

It has been widely recognized that estimating a dynamic model coefficient directly from an expression such as Eq. 8 is undesirable because the resulting coefficient values can exhibit rapid spatial variation. This violates the assumption made in removing the coefficient from test filtering operations and can negatively impact the stability of a simulation. Therefore, some form of spatial averaging is usually employed to evaluate a dynamic coefficient such as averaging over homogeneous directions of the flow (Germano et al., 1991), also referred to here as Germano averaging. By viewing points along a homogeneous direction as members of a statistical sample, this averaging can be associated with least squares line fitting (Pierce and Moin, 1998). Taking Eq. 8 and the case of a planar jet, the least squares fit over homogeneous directions approach yields $\mathscr{C}_\tau$ as

$$\mathscr{C}_\tau(x,y) = \frac{\langle XY \rangle_z}{\langle XX \rangle_z} \tag{14}$$

where $\langle \cdot \rangle_z$ indicates an average taken over the homogeneous z direction of the flow.

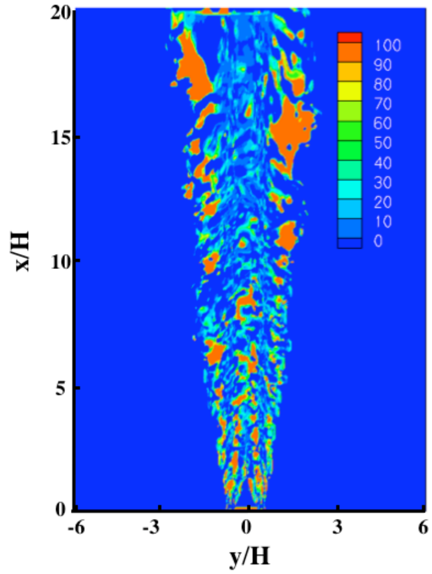
Fig. 1 shows values of $\mathscr{C}_\tau$ predicted for the planar jet case using Germano averaging, Eq. 14. The model coefficient shows rapid fluctuations between high and low values. Points along a spanwise averaging line are statistically equivalent in the sense of long time averages. At any given time step, however, these points can represent quite different flow conditions as the instantaneous locations of turbulent structures vary. The dynamic dissipation rate model also inherits the fluctuations of the dynamic eddy diffusivity model, whose coefficient $\mathscr{C}_Z$ is obtained using the same kind of spanwise averaging.

The predictions of the dynamic model using Germano averaging are compared to exact $\widetilde{\varepsilon_Z}$ values in Fig. 4. While there is some level of qualitative agreement, the dissipation rate is overpredicted near the inflow boundary. Additionally, the structures of the modeled dissipation rate are more fragmentary than those of the exact quantity.

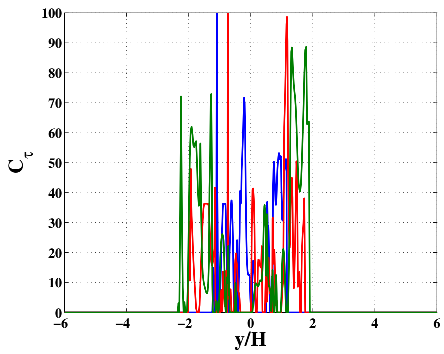
Conditional Averaging

In HIT, all points in the flow are statistically equivalent. Under the Germano averaging approach, averages are taken over the entire flow domain and a single coefficient is predicted at each time step. However, the relationship between $\widetilde{\varepsilon_Z}$ and Z_v/τ_Z seems to be more complex than that expressed by a global linear fit. The quantity

$$\langle \widetilde{\varepsilon_Z} | Z_v/\tau_Z \rangle \tag{15}$$



(a)



(b)

Figure 1. Prediction of $\mathscr{C}_\tau$ using Eq. 14. (a) Contours of $\mathscr{C}_\tau$ in xy-plane. (b) Instantaneous profiles of $\mathscr{C}_\tau$ at streamwise locations x/H of 3.33 (blue), 6.67 (red), and 13.33 (green).

where $\widetilde{\varepsilon}_Z$ is computed from a fully resolved scalar field using Eq. 2, is a valuable gauge of a dissipation rate model's accuracy. This is a specific case of the fact that the conditional mean of A conditioned on B, $\langle A|B\rangle$ is the minimum mean square error predictor of A given knowledge only of B (Deutsch, 1965). In a priori analysis, the conditional mean, Eq. 15, allows the deterministic predictions of a subfilter model to be compared quantitatively to exact subfilter quantities, which are random with respect to the filtered field. Fig. 2 shows the conditional mean, Eq. 15, computed from 512^3 DNS data. Clearly, its curved shape cannot be replicated by a single value of $\mathscr{C}_\tau$. To emphasize this point, Fig. 2 also shows the least squares line fitted to the exact dissipation, which is the ideal outcome of the dynamic model evaluated with Germano averaging in HIT.

Based on this observation, we propose an alternative averaging approach using conditional averaging on Z_v/τ_Z. Additionally, we restrict the average to those points for which $XY > 0$, i.e. points whose values of X and Y are consistent

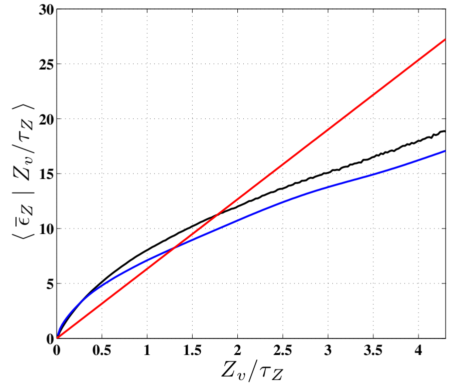


Figure 2. Conditional means of subfilter scalar dissipation from 512^3 DNS of homogeneous isotropic turbulence using exact dissipation, Eq. 2 (black); least squares linear fit to exact dissipation (red); dynamic model plus Eq. 16 (blue).

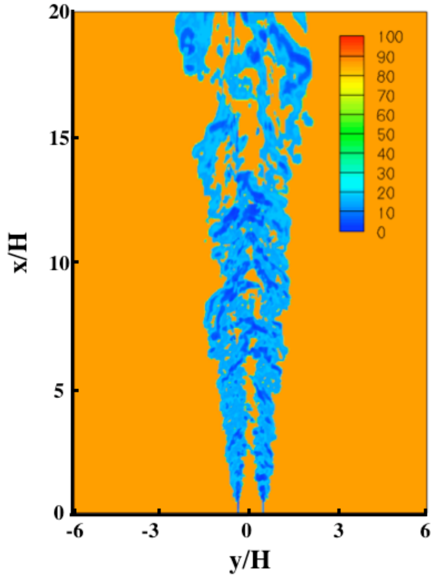
with a positive value of $\mathscr{C}_\tau$. Only those points which conform to the hypotheses of Eq. 8 are thus used to inform the prediction of $\mathscr{C}_\tau$. This conditional averaging approach can be written as

$$\mathscr{C}_\tau = \frac{\langle XY|Z_v/\tau_Z, XY > 0\rangle}{\langle XX|Z_v/\tau_Z, XY > 0\rangle} \tag{16}$$

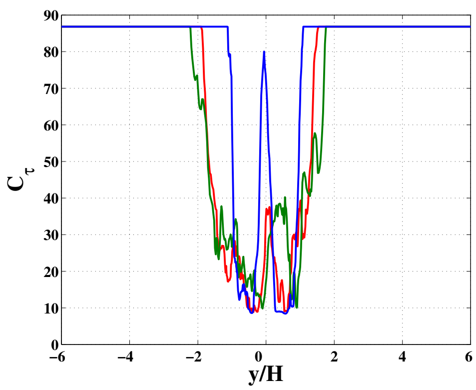
and predicts $\mathscr{C}_\tau$ as a function of Z_v/τ_Z. A variety of methods exist for computing conditional averages such as those in Eq. 16, the simplest probably being the histogram approach in which data are grouped into bins and an average is computed over each bin. Fig. 2 shows the results of applying Eq. 16 in HIT. The agreement with the conditional mean of the exact dissipation is very good. Fifty bins, spaced logarithmically in Z_v/τ_Z, were used in the computation. Halving the number of bins was found to have little effect on predicted dissipation values.

The conditional averaging approach can be applied to flow configurations besides HIT. Because all points in the flow are not statistically equivalent, the notion of a conditional average must be interpreted somewhat loosely. Conditional averaging could be carried out over homogeneous flow directions only, resulting in $\mathscr{C}_\tau$ values that are explicitly dependent on spatial location as well as on the conditioning variable Z_v/τ_Z. However, this can severely limit the sample size for estimating coefficients. Rather, we argue that it is reasonable for the conditional coefficient calculation to amalgamate points over the entire flow domain, regardless of the flow geometry. A basic principle of LES modeling is that geometry-specific features of the flow are captured by the resolved fields while subfilter scale motions are not directly dependent on the large scales. From this viewpoint, a subfilter model coefficient should not require explicit geometrical dependence if local flow conditions are adequately accounted for by the choice of conditioning variable.

Predictions of $\mathscr{C}_\tau$ using Eq. 16 are shown in Fig. 3. The nonzero coefficient value predicted in laminar regions is an artifact of the binning method, which did not distinguish between very small and zero values of Z_v/τ_Z. However, because



(a)



(b)

Figure 3. Prediction of $\mathscr{C}_\tau$ using Eq. 16. (a) Contours of $\mathscr{C}_\tau$ in a representative xy-plane. (b) Instantaneous profiles of $\mathscr{C}_\tau$ at streamwise locations x/H of 3.33 (blue), 6.67 (red), and 13.33 (green).

Z_v/τ_Z is zero in those areas the model, Eq. 5, still properly predicts zero dissipation. Twenty logarithmically spaced bins were used in the computation of $\mathscr{C}_\tau$. The dynamic eddy viscosity coefficient $\mathscr{C}_Z$ was found using a local averaging procedure over test filter volumes. This approach was used to eliminate any effect, even indirect, of averaging over homogeneous directions from the prediction of $\mathscr{C}_\tau$. The utility of a conditional averaging method for $\mathscr{C}_Z$ remains open to investigation.

Fig. 3 shows the spatial distribution of $\mathscr{C}_\tau$ predicted using conditional averaging, Eq. 16. The variation is smoother than that seen in Fig. 1 and more clearly related to the turbulent structure of the jet. The subfilter dissipation rate values obtained using this model implementation are plotted in Fig. 4. The conditional averaging approach gives a good approximation to the exact dissipation near the jet inflow (Fig. 5). Dissipation is overpredicted downstream. However, the accuracy

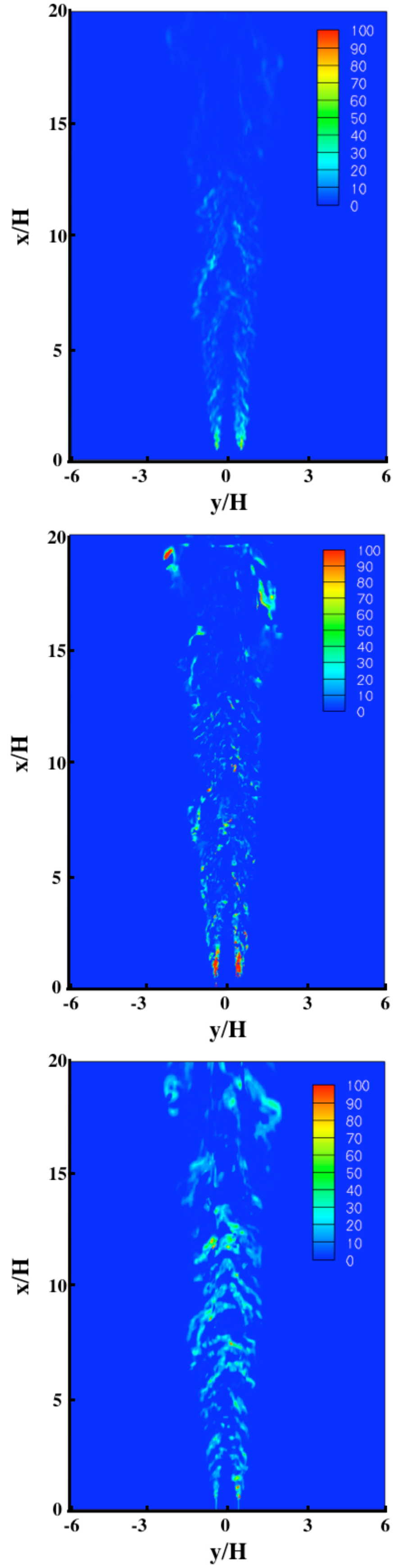


Figure 4. Contours of $\widetilde{\varepsilon_Z}$: exact, Eq. 2 (top); dynamic model plus Eq. 14 (middle); dynamic model plus Eq. 16 (bottom).

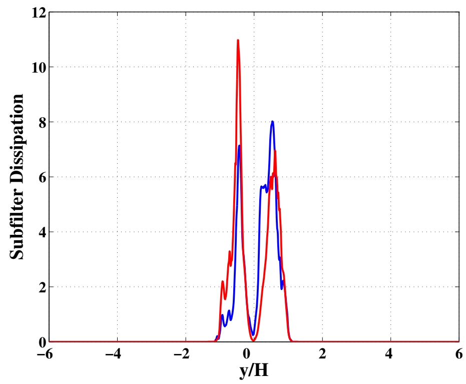


Figure 5. Instantaneous profiles of $\widetilde{\varepsilon_Z}$ at streamwise location $x/H = 3.33$: exact dissipation, Eq. 2 (red) and dynamic model plus Eq. 16 (blue).

of the dynamic dissipation rate model is contingent on the accuracy of other closures of the VTE, such as the variance production term. In unclosed form, the production term is given by the product of the subfilter scalar flux and the filtered scalar gradient and can be positive or negative. The closed form of the production term, as in Eq. 3, follows from substitution of an eddy diffusion model for the subfilter scalar flux. The production model underpredicts the magnitude of the true production when it is positive and cannot capture regions of negative production. Production modeling errors are actually larger than dissipation modeling errors at these locations. Note that the term P, Eq. 11, in the dynamic model is the change in production between the test and filter scales. Therefore, if the model behaves consistently at the two scales it remains possible to predict the value of this difference more accurately than the actual magnitude of production.

CONCLUSIONS

A dynamic procedure for non-equilibrium modeling of subfilter scalar dissipation rate was developed by applying the variance transport equation at two scales. The effects of different averaging procedures for estimation of the model coefficient were considered. Specifically, Germano averaging over homogeneous flow directions was compared with a novel conditional averaging approach in homogeneous isotropic turbulence and in a planar jet configuration. The choice of averaging procedure had significant impact on dynamic modeling outcomes and affected the spatial patterning of the predicted dissipation fields as well as the magnitude of the modeled dissipation values. Upstream, the conditional averaging approach yielded good agreement with exact dissipation values but showed lower accuracy downstream. However, the dissipation rate modeling errors were smaller than errors in the production term at these locations.

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