Modeling of the subfilter scalar dissipation rate using the concept of optimal estimators

G. Balarac,[1,a)] H. Pitsch,[1] and V. Raman[2]
[1]*Center for Turbulence Research, Stanford University, Stanford, California 94305, USA*
[2]*The University of Texas at Austin, Austin, Texas 78712, USA*

(Received 17 April 2008; accepted 5 August 2008; published online 5 September 2008)

In this work, modeling of the subfilter scalar dissipation rate is addressed. First, the best set of quantities to write a model is determined using the concept of optimal estimators. This study shows that the best approach is to assume a proportionality between the turbulent time scale and turbulent scalar mixing time scale. It is shown that the turbulent time scale should be defined by the subfilter kinetic energy. To define the coefficient appearing in this model, a dynamic determination based on a global subfilter equilibrium assumption between the dissipation and the production terms leads to the best results. © *2008 American Institute of Physics*. [DOI: 10.1063/1.2976818]

In large eddy simulation (LES), a spatial filtering operation is applied to an instantaneous field, f, to separate the large-scale quantity, $\bar{f}$, from the small scales. Transport equations are solved only for the large-scale quantities, and the contribution of the unresolved small-scale features of the flow needs to be modeled. In the case of hydrodynamic problems, this technique is now commonly used and many models have been proposed to close the filtered Navier–Stokes equations.[1] However, LES applied to combustion problems is a relatively new field.[2] The main difficulty is that combustion itself is directly influenced mostly by the small scales. Most of the currently available combustion models use mixture fraction, Z, a conserved scalar, to describe local variations in fuel-air ratio. Two quantities that are important in the statistical description of the mixture fraction are the filtered mixture fraction, $\bar{Z}$, and its variance, $Z_v=\overline{ZZ}-\bar{Z}\bar{Z}$. Transport equations can be derived for both quantities, but the dissipation rate of the scalar variance, appearing in the variance equation, requires modeling. Since the dissipation of mixture-fraction variance leads to mixing of fuel and air on the molecular level, this process enables chemical reactions. For this reason, the scalar dissipation has a special role in combustion modeling. In fact, it can be shown[3] that the chemical source term is directly proportional to the scalar dissipation rate as long as the chemistry is fast enough. This quantity therefore appears in essentially all models for nonpremixed combustion, such as the flamelet model, the conditional moment closure model, and the transported PDF model (see Pitsch[2] for a review). The transport equation of the subfilter scalar variance is[4]

$$\frac{\partial Z_v}{\partial t}+u_i\frac{\partial Z_v}{\partial x_i}=D\frac{\partial^2 Z_v}{\partial x_i^2}-\frac{\partial}{\partial x_i}\left(\overline{u_iZ^2}-\bar{u}_i\overline{Z^2}-2\bar{Z}T_i\right)-2T_i\frac{\partial\bar{Z}}{\partial x_i}+2D\frac{\partial\bar{Z}}{\partial x_i}\frac{\partial\bar{Z}}{\partial x_i}-2D\overline{\frac{\partial Z}{\partial x_i}\frac{\partial Z}{\partial x_i}}, \quad (1)$$

where D is the molecular diffusivity and $T_i=\overline{u_iZ}-\bar{u}_i\bar{Z}$ is the subfilter scalar flux. The subfilter scalar dissipation rate is then defined by

$$\bar{\varepsilon}=2D\left(\overline{\frac{\partial Z}{\partial x_i}\frac{\partial Z}{\partial x_i}}-\frac{\partial\bar{Z}}{\partial x_i}\frac{\partial\bar{Z}}{\partial x_i}\right). \quad (2)$$

Since only the first term in Eq. (2) needs to be modeled in LES, it is helpful to define the filtered scalar dissipation rate as

$$\bar{\chi}=2D\overline{\frac{\partial Z}{\partial x_i}\frac{\partial Z}{\partial x_i}}. \quad (3)$$

Scalar dissipation, similar to viscous momentum dissipation, occurs predominantly at the small scales. Since LES does not directly resolve these scales, modeling of $\bar{\varepsilon}$ is particularly challenging.

In this work, first the commonly used models are studied in *a priori* tests. Using the concept of optimal estimator,[5] the best set of quantities to use when writing a model for $\bar{\varepsilon}$ is then determined. Finally, different methods to determine the coefficient that appears in this model are investigated.

Direct numerical simulation (DNS) of forced isotropic turbulence is used to perform the *a priori* tests. A standard pseudospectral code (e.g., Kuczaj and Geurts[6]) is used with 512^3 points. The domain size is larger than four integral scales, while the smallest length scales are resolved according to the conditions specified in Pope.[7] The Taylor-scale Reynolds number is around 180. The molecular Schmidt number is set to 0.7. The same data have been used already to study the modeling of the subfilter scalar variance.[8] In the *a priori* tests, a box filter is used to define LES quantities. In the following discussion, the filter size Δ is expressed as a multiple of the Kolmogorov scale η. A large range of ratios of the filter scale to Kolmogorov scale has been tested with a filter sizes range from the dissipative region to the top of the inertial region.

While performing *a priori* based model evaluation, an important consideration is the choice of an error measure. A reliable measure of error can be obtained based on the optimal estimation theory.[5] Let us consider a variable set ϕ used to model the scalar dissipation rate as follows:

a)Electronic mail: balarac@stanford.edu.

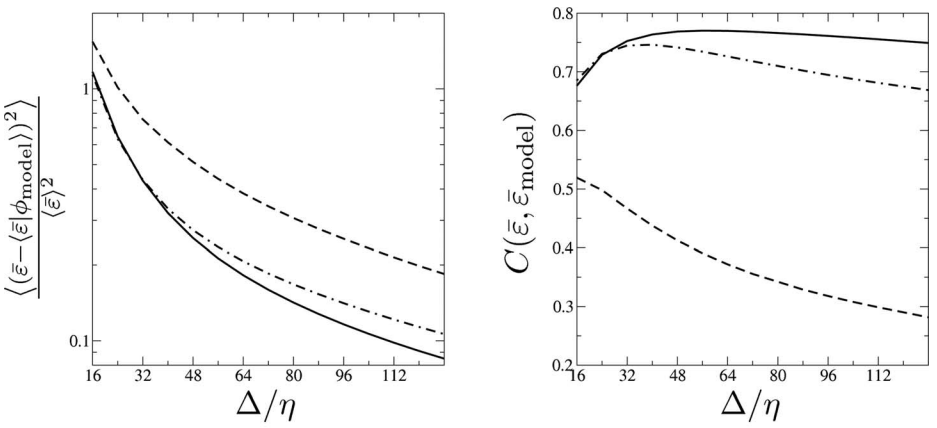

FIG. 1. (a) Irreducible error as function of filter size; (b) correlation between exact and modeled subfilter dissipation rate. LEA model (– – –), SRT model (– · –), and SKE model (——).

$$\bar{\varepsilon} = g(\phi), \tag{4}$$

where g refers to a mapping function operating on the variable set. The conditional mean $\langle\bar{\varepsilon}|\phi\rangle$ is the optimal estimator of $\bar{\varepsilon}$ using ϕ as variables. Then, $\langle(\bar{\varepsilon}-\langle\bar{\varepsilon}|\phi\rangle)^2\rangle$ is the least quadratic error that can be obtained using the model based on ϕ. This error is called the irreducible error for the chosen variable set, which can be reduced only by changing the set of variables used in the model. About the practical implementation, a histogram method has been used to compute the conditioned means. It has been checked that the choice of the number of cells has not influenced the results.

The most commonly used model for evaluating the filtered scalar dissipation rate is based on the eddy diffusivity assumption (EDA).[9,10] For the sake of the following discussion, this formulation is termed the EDA model:

$$\bar{\chi}_{\text{EDA}} = 2(D + D_T)\frac{\partial\bar{Z}}{\partial x_i}\frac{\partial\bar{Z}}{\partial x_i}, \tag{5}$$

where $D_T = \nu_T/Sc_T$ is the eddy diffusivity defined by the eddy viscosity, ν_T, and the eddy Schmidt number, Sc_T. In fact, this model comes from a local equilibrium assumption (LEA) between the dissipation and the production terms in the transport equation of the subfilter scalar variance, Eq. (1). This assumption leads first to a more general form, termed here the LEA model,[10]

$$\bar{\chi}_{\text{LEA}} = 2D\frac{\partial\bar{Z}}{\partial x_i}\frac{\partial\bar{Z}}{\partial x_i} - 2T_i\frac{\partial\bar{Z}}{\partial x_i}. \tag{6}$$

The LEA model is written for the subfilter dissipation rate as

$$\bar{\varepsilon}_{\text{LEA}} = -2T_i\frac{\partial\bar{Z}}{\partial x_i}. \tag{7}$$

The subfilter scalar flux, T_i, is not known in LES but can be modeled by an eddy diffusivity assumption,[11,12] which then leads to the EDA model. In this work, to focus only on the modeling of the scalar dissipation, T_i will be evaluated directly from the DNS data. The set of quantities used in the LEA model is then $\phi_{\text{LEA}} = \{-2T_i(\partial\bar{Z}/\partial x_i)\}$.

In Reynolds-averaged approach, an algebraic relation linking scalar dissipation rate to the local mixture-fraction variance is commonly used.[13] A similar approach can be used for LES as well. Here, the subfilter scalar mixing time scale, $Z_v/\bar{\varepsilon}$, is assumed to be proportional to the subfilter turbulent time scale, τ:

$$\bar{\varepsilon} = C_\tau\frac{Z_v}{\tau}, \tag{8}$$

where C_τ is the time scale ratio. The turbulence time scale can be first defined as $\tau = 1/|\bar{S}|$, where $|\bar{S}|$ is the magnitude of the large-scale strain rate tensor (SRT) $|\bar{S}| = (2\bar{S}_{ij}\bar{S}_{ij})^{1/2}$, with

$$\bar{S}_{ij} = \frac{1}{2}\left(\frac{\partial\bar{u}_i}{\partial x_j} + \frac{\partial\bar{u}_j}{\partial x_i}\right). \tag{9}$$

The SRT model is then defined as

$$\bar{\varepsilon}_{\text{SRT}} = C_{\tau,\text{SRT}}Z_v|\bar{S}|, \tag{10}$$

with the following set of parameters $\phi_{\text{SRT}} = \{Z_v|\bar{S}|\}$. Note that, considering the eddy viscosity defined by a conventional Smagorinsky closure,[14] $\nu_T = (C_S\Delta)^2|\bar{S}|$, the set of parameters also follows from evaluating the turbulent time scale by[15] Δ^2/ν_T (or by[16] Δ^2/D_T).

The characteristic turbulent time scale can also be defined as $\tau = \Delta/k^{1/2}$ with the subfilter kinetic energy (SKE), $k = \frac{1}{2}(\overline{u_iu_i} - \bar{u}_i\bar{u}_i)$. We define the SKE model by[17]

$$\bar{\varepsilon}_{\text{SKE}} = C_{\tau,\text{SKE}}\frac{Z_vk^{1/2}}{\Delta} \tag{11}$$

and its set of quantities is $\phi_{\text{SKE}} = \{Z_vk^{1/2}/\Delta\}$. The quantities Z_v and k are unknown quantities in LES. Several possibilities are available to evaluate these terms, using direct modeling[8,18] or transport equations.[4,19] In this work, we evaluate Z_v and k from the DNS data to focus on the modeling of $\bar{\varepsilon}$.

To determine the most suitable model for the subfilter scalar dissipation rate, we will first determine the best set of quantities to be used in the model. The best set of quantities to write a model is the set of quantities that results in the smallest quadratic error of the optimal estimator, i.e., the smallest irreducible error. The irreducible error for all models is given in Fig. 1(a). The errors have been normalized by the subfilter scalar dissipation rate. Since the subfilter scalar dissipation rate is very small for smaller filter size, the nor-

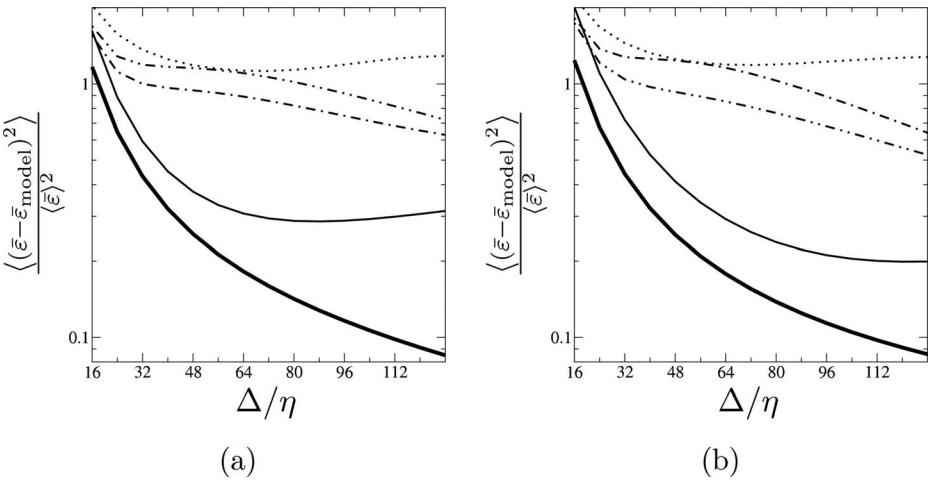

FIG. 2. Total quadratic error of the SKE model as function of filter size computed with the constants $C_{\tau,1}$ (– · · –), $C_{\tau,2}$ (– · –), $C_{\tau,3}$ (· · · ·), and $C_{\tau,4}$ (——). The irreducible error of $\bar{\varepsilon}_{\text{SKE}}$ is given by the bold line. (a) Forced turbulence and (b) decaying turbulence ($R_\lambda \approx 125$).

malized errors are high for the smaller filter sizes and decrease after. It is clear that the models based on a turbulent time scale lead to smaller irreducible errors compared to the LEA model. Since the exact value of the subfilter scalar flux is considered in the *a priori* tests, the results of the LEA model depend only on the validity of the local equilibrium assumption between production and dissipation, irrespective of the model used for the production term. Thus, the large irreducible errors of the LEA model reveal that the equilibrium assumption is locally not verified.[20] The set of quantities ϕ_{SKE} gives the smallest irreducible error. This shows that an evaluation of the turbulence time scale based on the subfilter kinetic energy is more suitable. To confirm that the SKE model is the best candidate to evaluate $\bar{\varepsilon}$, we have computed the correlation between the subfilter dissipation rate of the DNS and the different models [Fig. 1(b)]. Note that the correlation is independent of the model coefficient value. Confirming the results from Fig. 1(a), the SKE model is strongly correlated with the exact subfilter dissipation and its correlation is always higher than that of the other models. For the smallest filter sizes, the results are similar for both the SKE and SRT models. It is because when the filter size is in the dissipative region, a local balance between energy production and dissipation is verified[20] allowing to link k with $|\bar{S}|$ as done by Yoshizawa's model,[21] $k=C\Delta^2|\bar{S}|^2$ with C a constant. Note that the correlation of the LEA model is exactly the correlation between the production term and the dissipation term in the transport equation of the subfilter scalar variance, Eq. (1). This confirms that the equilibrium assumption is not satisfied locally.

Since the set of quantities ϕ_{SKE} leads to the smallest irreducible error, the SKE model appears to be the most promising model to evaluate the subfilter scalar dissipation rate. The remaining challenge is then to evaluate the coefficient $C_{\tau,\text{SKE}}$ in Eq. (11). Schmidt and Schumann[17] proposed the use of the time scale ratio a value of $C_{\tau,1}=2.02$ considering an inertial range kinetic energy spectrum and an inertial-convective range scalar variance spectrum. Another approach is to evaluate a turbulent time scale proportional to Δ^2/ν_T and a turbulent-mixing time scale proportional to Δ^2/D_T. Assuming the same proportional coefficient for both time scales, the ratio is given by $C_{\tau,2}=D_T/\nu_T=1/Sc_T$. In the following tests, we evaluate the eddy viscosity and the eddy diffusivity from the DNS data as[12]

$$\nu_T=-\frac{\langle T_{ij}\bar{S}_{ij}\rangle}{2\langle\bar{S}_{kl}\bar{S}_{kl}\rangle},\quad D_T=-\frac{\left\langle T_i\dfrac{\partial\bar{Z}}{\partial x_i}\right\rangle}{2\left\langle\dfrac{\partial\bar{Z}}{\partial x_j}\dfrac{\partial\bar{Z}}{\partial x_j}\right\rangle},$$

where $T_{ij}=\overline{u_iu_j}-\bar{u}_i\bar{u}_j$ is the subfilter stress tensor.

A dynamic approach was considered by Wong[22] to compute the coefficient for the subfilter kinetic energy dissipation rate. A similar approach has already been used for the subfilter scalar dissipation rate.[15] To determine $C_{\tau,3}$, the first step is to filter Eq. (11) with a test filter of size $\hat{\Delta}=2\Delta$ denoted by $\hat{\cdot}$, assuming that the model coefficient varies slowly in space. The second step is to write the SKE model with the same coefficient for the test filter. We can then write $L_d=C_{\tau,3}M_d$ with

$$L_d=2D\left(\widehat{\frac{\partial\bar{Z}}{\partial x_i}\frac{\partial\bar{Z}}{\partial x_i}}-\frac{\partial\hat{\bar{Z}}}{\partial x_i}\frac{\partial\hat{\bar{Z}}}{\partial x_i}\right)\quad\text{and}\quad M_d=\frac{Z_{v,T}k_T^{1/2}}{\hat{\Delta}}-\frac{\widehat{Z_vk^{1/2}}}{\Delta},\tag{12}$$

where $Z_{v,T}=\widehat{\bar{Z}\bar{Z}}-\hat{\bar{Z}}\hat{\bar{Z}}$ and $k_T=\frac{1}{2}(\widehat{\bar{u}_i\bar{u}_i}-\hat{\bar{u}}_i\hat{\bar{u}}_i)$. To evaluate $Z_{v,T}$ and k_T from LES data, we can write these quantities as $Z_{v,T}=\hat{Z}_v+\widehat{\bar{Z}\bar{Z}}-\hat{\bar{Z}}\hat{\bar{Z}}$ and $k_T=\hat{k}+\frac{1}{2}(\widehat{\bar{u}_i\bar{u}_i}-\hat{\bar{u}}_i\hat{\bar{u}}_i)$. $C_{\tau,3}$ is then obtained using a least-squares averaging procedure.[23] However, it should be noted here that this approach is already not expected to be useful. For any filter size with the filter located in the inertial subrange, the subfilter contribution to dissipation is much larger than the resolved contribution. Hence, both L_d and M_d tend to zero and the determination of $C_{\tau,3}$ becomes singular.

Finally, we propose a new approach based on a global subfilter equilibrium assumption. As already shown, the subfilter equilibrium between dissipation and production terms is not satisfied locally, but under certain conditions, we can expect this condition to hold on an average. To determine $C_{\tau,\text{SKE}}$, we propose to use a subfilter equilibrium assumption

as in Eq. (7), but with a suitable average. Using Eq. (7), the global subfilter equilibrium assumption is written as

$$\langle \bar{\varepsilon} \rangle = -2 \left\langle T_i \frac{\partial \bar{Z}}{\partial x_i} \right\rangle. \tag{13}$$

This is similar to the method proposed by You and Moin[24] to compute the coefficient of an eddy viscosity model. Using the SKE model for $\bar{\varepsilon}$ in Eq. (13), the coefficient $C_{\tau,4}$ is defined as

$$C_{\tau,4} = -2\Delta \frac{\langle T_i(\partial \bar{Z}/\partial x_i)\rangle}{\langle k^{1/2} Z_v \rangle}. \tag{14}$$

The performance of the four different ways to compute the model coefficient is assessed next. Figure 2(a) shows the total quadratic error of each model, which is defined as $\langle(\bar{\varepsilon} - \bar{\varepsilon}_{\text{model}})^2\rangle$. These errors are compared to the irreducible error of the SKE model. The coefficient $C_{\tau,4}$ computed by Eq. (14) leads to the smallest total quadratic error and it stays close to the irreducible error. As expected, the traditional dynamic procedure for the dissipation rate is very inaccurate, since the most important contribution to the dissipation rate occurs at the small scales and the resolved contribution at a higher filter size cannot retain enough information. This has already been pointed out by Pierce and Moin.[10] The new model is the most accurate for the considered test case, and this model assumes that subfilter production equals dissipation. Although the production term in Eq. (13) is actually just an energy transfer into the subfilter scales, the condition that large-scale production globally equals dissipation is enforced in stationary forced isotropic turbulence. For this reason, it is important to demonstrate that the method is still accurate for decaying isotropic turbulence, for which the large-scale production is zero. Figure 2(b) shows the total error of each model in decaying turbulence. $C_{\tau,4}$ again leads to the smallest total error. The reason is that the assumption in Eq. (13) does not require a global equilibrium, but only an equilibrium on the subfilter scales, which seems to be satisfied on an average, even in the absence of large-scale production. This shows also that the results are the same for different Reynolds number. This model should thus be applicable in various configurations.

In conclusion, the concept of optimal estimator has been used to determine the best way to model the subfilter scalar dissipation rate. It appears that a model based on the ratio of turbulent to scalar time scale, where the turbulent time scale is evaluated from the subfilter kinetic energy gives the lowest irreducible error. It is shown that the smallest quadratic error is achieved when the model coefficient representing the time scale ratio is determined with the assumption that for a suitable ensemble, the subfilter equilibrium holds on average. This average could be evaluated over statistically homogeneous directions, or, for flows in complex geometry, as an average over flow pathlines as proposed by Meneveau *et al.*[25] with the Lagrangian dynamic procedure. On the other hand, the "global subfilter equilibrium assumption" has already be used by You and Moin[24] with entire volume average to the determination of dynamic model coefficient. This volume averaging can be appeared as an alternative to the Lagrangian procedure. Future works will be a study of the combination of various modeling errors and the combination with numerical errors with a particular focus to dissociate these various sources of error. The goal will be to understand the part of each error in an *a posteriori* LES.

The authors are thankful to L. Jacoutot and O. Desjardins for their fruitful comments on a draft of this manuscript. The authors gratefully acknowledge funding from NASA and the Air Force Office of Scientific Research.

[1] C. Meneveau and J. Katz, "Scale-invariance and turbulence models for large-eddy simulation," Annu. Rev. Fluid Mech. **32**, 1 (2000).
[2] H. Pitsch, "Large-eddy simulation of turbulent combustion," Annu. Rev. Fluid Mech. **38**, 453 (2006).
[3] R. W. Bilger, "The structure of diffusion flames," Combust. Sci. Technol. **13**, 155 (1976).
[4] C. Jiménez, F. Ducros, B. Cuenot, and B. Bédat, "Subgrid scale variance and dissipation of a scalar field in large eddy simulations," Phys. Fluids **13**, 1748 (2001).
[5] A. Moreau, O. Teytaud, and J. P. Bertoglio, "Optimal estimation for large-eddy simulation of turbulence and application to the analysis of subgrid models," Phys. Fluids **18**, 105101 (2006).
[6] A. K. Kuczaj and B. J. Geurts, "Mixing in manipulated turbulence," J. Turbul. **7**, 1 (2006).
[7] S. B. Pope, *Turbulent Flows* (Cambridge University Press, Cambridge, England, 2000).
[8] G. Balarac, H. Pitsch, and V. Raman, "Development of a dynamic model for the subfilter scalar variance using the concept of optimal estimators," Phys. Fluids **20**, 035114 (2008).
[9] S. S. Girimaji and Y. Zhou, "Analysis and modeling of subgrid scalar mixing using numerical data," Phys. Fluids **8**, 1224 (1996).
[10] C. D. Pierce and P. Moin, "A dynamic model for subgrid-scale variance and dissipation rate of a conserved scalar," Phys. Fluids **10**, 3041 (1998).
[11] P. Moin, K. Squires, W. Cabot, and S. Lee, "A dynamic subgrid-scale model for compressible turbulence and scalar transport," Phys. Fluids A **3**, 2746 (1991).
[12] C. Brun, G. Balarac, C. B. da Silva, and O. Métais, "Effects of molecular diffusion on the subgrid-scale modelling of passive scalars," Phys. Fluids **20**, 025102 (2008).
[13] J. P. H. Sanders and I. Gökalp, "Scalar dissipation rate modelling in variable density turbulent axisymmetric jets and diffusion flames," Phys. Fluids **10**, 938 (1998).
[14] M. Germano, U. Piomelli, P. Moin, and W. H. Cabot, "A dynamic subgrid-scale eddy viscosity model," Phys. Fluids A **3**, 1760 (1991).
[15] C. Pera, J. Réveilon, L. Vervisch, and P. Domingo, "Modeling subgrid scale mixture fraction variance in LES of evaporating spray," Combust. Flame **146**, 635 (2006).
[16] P. J. Colucci, F. A. Jaberi, P. Givi, and S. B. Pope, "Filtered density function for large eddy simulation of turbulent reacting flows," Phys. Fluids **10**, 499 (1998).
[17] H. Schmidt and U. Schumann, "Coherent structure of the convective boundary layer derived from large-eddy simulations," J. Fluid Mech. **200**, 511 (1989).
[18] B. Knaepen, O. Debliquy, and D. Carati, "Subgrid-scale energy and pseudo pressure in large-eddy simulation," Phys. Fluids **14**, 4235 (2002).
[19] S. Ghosal, T. Lund, P. Moin, and K. Akselvoll, "A dynamic localization model for large-eddy simulation of turbulent flows," J. Fluid Mech. **286**, 229 (1995).
[20] C. B. da Silva and J. C. F. Pereira, "On the local equilibrium of the subgrid scales: The velocity and scalar fields," Phys. Fluids **17**, 108103 (2005).
[21] A. Yoshizawa, "Statistical theory for compressible turbulent shear flows, with the application to subgrid modeling," Phys. Fluids **29**, 2152 (1986).
[22] V. C. Wong, "A proposed statistical-dynamic closure method for the linear or nonlinear subgrid-scale stresses," Phys. Fluids A **4**, 1080 (1992).
[23] D. K. Lilly, "A proposed modification of the Germano subgrid-scale closure method," Phys. Fluids A **4**, 633 (1992).
[24] D. You and P. Moin, "A dynamic global-coefficient subgrid-scale eddy-viscosity model for large-eddy simulation in complex geometries," Phys. Fluids **19**, 065110 (2007).
[25] C. Meneveau, T. Lund, and W. Cabot, "A Lagrangian dynamic subgrid-scale model of turbulence," J. Fluid Mech. **319**, 353 (1996).