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NUMERICAL ERRORS IN SCALAR VARIANCE MODELS FOR LARGE EDDY SIMULATION

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ABSTRACT

The subfilter scalar variance is an important quantity in conserved scalar models for large eddy simulation of turbulent combustion, where it indicates the degree of small scale mixing between fuel and oxidizer. Simulation predictions of chemical species concentrations are sensitive to the accuracy of the variance model, including the numerical accuracy with which the model is evaluated. *A priori* analysis shows that both dynamic algebraic models and transport equation models for the variance incur significant numerical error when calculated using finite difference methods. Furthermore, the amount of error cannot be reliably characterized by the order of accuracy of the finite difference scheme.

Errors in the filtered scalar field also contribute to the error in the variance estimation. In particular, the variance values predicted by a dynamic model are highly dependent on the evolution of the smallest resolved scales, which in turn are greatly influenced by the numerical treatment of the diffusive term. In *a posteriori* tests, a simple expansion of the term is found to improve the accuracy of the scalar evolution and, thereby, increase the accuracy of dynamic model predictions of the variance. In contrast to the *a priori* results, the combined numerical errors of the scalar equation and variance model evaluation cause the magnitude of modeled variance values to increase as the order of accuracy of the finite difference scheme decreases.

INTRODUCTION

Large eddy simulation (LES) has emerged as an important tool for modeling turbulent combustion. Large scale motions are nominally resolved in LES, while small scales processes must be described using models. Although combustion itself takes place at the smallest scales, the combustion rate is limited by the large-scale mixing process, which is predicted well by LES. It has been argued that this factor increases the over-all accuracy of LES methods relative to RANS-based approaches. With that said, proper representation of small scale mixing is essential for accurate LES of combustion.

In LES, the true flow field is separated into a filtered field (denoted by $\overline{\cdot}$) and a subfilter field using a lowpass filtering kernel. Combustion is typically modeled using mixture fraction, which is a conserved scalar. Specifically, the filtered mixture fraction and the variance of mixture fraction are needed to prescribe the subfilter thermochemical state.The subfilter variance for mixture fraction Z is then defined as $\overline{Z'^2} = \overline{Z^2} - \overline{Z}^2$, and needs to be modeled since $\overline{Z^2}$ is not generally available from the LES computation. Several models for the variance have been proposed, prompting comparisons of these models in terms of their ability to capture the physics of small scale mixing. When the results of these idealized analyses are applied to actual simulations, it is implicitly assumed that numerical errors are a secondary effect. This is, from the start, a tenuous assumption since the nonlinearity of combustion models means that even small errors in the variance can produce large errors in species concentrations. Additionally, in practical applications, LES is performed using grid-based filtering, so that the smallest filtered scales are poorly resolved by the computational mesh. These scales are important in determining modeled variance values, as described below, suggesting that the effects of nu-

merical error are critical.

Variance models can be grouped into two major categories: algebraic models and transport equation based models. Algebraic models assume that the local production and dissipation of scalar energy are always in balance, implying that physical transport of energy can be neglected (Balarac et al., 2008). In this work, the latter two models are considered. Here, the variance is modeled using a gradient-based scaling law (Pierce and Moin, 1998):

$$\overline{Z'^2} = C\Delta^2 \nabla\overline{Z} \cdot \nabla\overline{Z}, \tag{1}$$

where Δ is the filter-width and the model constant C is evaluated using a dynamic procedure. The coefficient is determined as a ratio between the Leonard term, which represents the scalar energy present at length scales between the filter scale and twice the filter scale, and a term that depends on gradients of the filtered scalar. The latter term takes slightly different forms in the original (Pierce and Moin, 1998) and modified (Balarac et al., 2008) dynamic models. While the local equilibrium assumption is questionable in even homogeneous isotropic flows, their relative ease of implementation has made these models popular. If the local equilibrium assumption has to be relaxed, then a transport equation for variance must be directly solved. Here, two choices exist: either the variance transport equation (VTE) or the second moment ($\overline{Z^2}$) transport equation (STE) may be used.

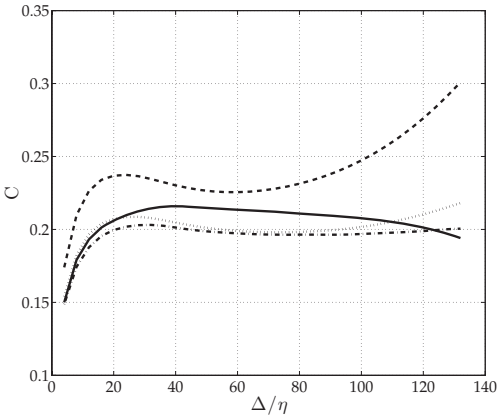
As a first step to understanding the consequences of numerical implementation on the aforementioned models, *a priori* tests were carried out using DNS data from a pseudospectral simulation of scalar mixing in forced isotropic turbulence. The findings of this analysis, which are summarized below, show that multiple sources of error within the subfilter model calculation can interact to produce unexpected outcomes. Numerical errors in the variance prediction can be large, even when sixth order accurate finite difference schemes are used. In an actual simulation, the numerical evolution of the scalar field also contributes to the error in the variance prediction. Thus, *a posteriori* tests were performed to complement and extend the *a priori* results. These show that proper treatment of the diffusive term of the filtered scalar treatment is required to avoid an accumulation of error near the filter cut-off scale, with significant impact on the variance prediction.

A PRIORI RESULTS

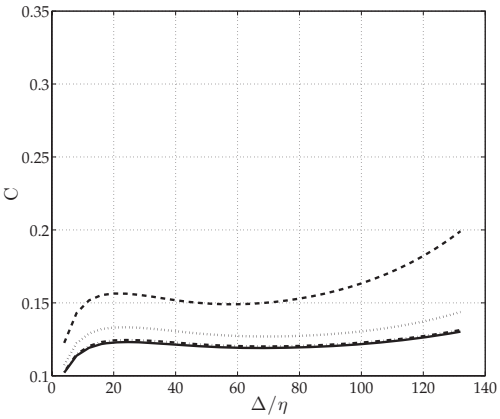
In the following *a priori* analysis of variance models, the effects of finite difference evaluation were emulated through the modified wavenumber representation of finite difference schemes (Kravchenko and Moin, 1997) and compared to model evaluations using the true wavenumber. Throughout, second order central (CD-2), fourth order central (CD-4) and sixth order Padé (P-6) schemes are considered.

Dynamic Models

The most overt source of error in the dynamic model (Eq. 1) is the evaluation of the gradient term. It is well known that finite difference approximations grossly underpredict the gradients in a turbulent flow. Ostensibly, the dynamic model should then underpredict the variance. However, the dynamic procedure used to compute the model coefficient also incurs numerical errors. These errors lead to an overprediction of the model coefficient relative to value determined by exact evaluation of the dynamic closure. Fig. 1 shows the original and modified dynamic model coefficients evaluated from DNS using the three different finite difference approximations. It can be seen that the second order central scheme, which is the least accurate of the schemes, predicts the highest model coefficient for all filter sizes considered. This overprediction partially offsets the error in the gradient estimation, thereby reducing the errors in the prediction of variance (Fig. 2(a)). It should be noticed that for the original dynamic model the use of finite differences actually changes the trends exhibited by the coefficient, while the effect on the modified dynamic model is limited to a scaling of the coefficient value. This difference is reflected in the model errors. Over a significant range of filter widths, the presence of numerical error actually improves the predictions of the original dynamic model. The modified dynamic model shows a more consistent behavior, in that increasing the accuracy of the numerical scheme increases the accuracy of the model over the full range of filter widths.



(a) Original dynamic model.

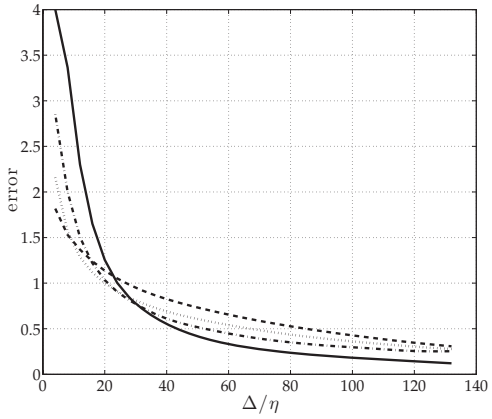


(b) Modified dynamic model.

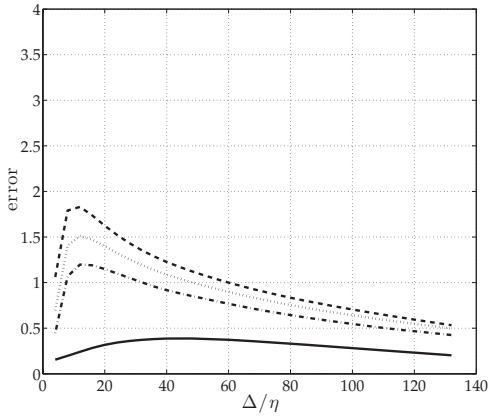
Figure 1: Dynamic model coefficient, computed using ensemble averaging over the entire domain, as a function of filter size and numerical scheme: (———) spectral (– – – –) CD-2 (·····) CD-4 and (—·—) P-6

Transport Equation Models

The second portion of *a priori* tests focus on transport equation based models. An obvious choice is the VTE model



(a) Original dynamic model.



(b) Modified dynamic model.

Figure 2: Quadratic errors of dynamic models $\langle(\overline{Z'^2}_{\text{model}} - \overline{Z'^2})^2\rangle/\langle\overline{Z'^2}\rangle^2$ for (———) spectral (– – – –) CD-2 (·····) CD-4, and (—·—) P-6 schemes.

which uses a transport equation for the variance. An aspect of the VTE that has received little attention originates in its derivation. Since $\overline{Z'^2}$ is not a conserved quantity, the VTE must be developed by manipulation of the $\overline{Z}$ equation through the chain rule rule. While this approach is analytically valid, it can be numerically problematic. For this discussion, we define the quantities

$$P_1 = 2\overline{Z}\frac{\delta\overline{u}_j\overline{Z}}{\delta x_j} \tag{2}$$

$$P_2 = \frac{\delta\overline{u}_j\overline{Z}^2}{\delta x_j} \tag{3}$$

and

$$Q_1 = 2\overline{Z}\frac{\delta}{\delta x_j}\left[(D+D_t)\frac{\delta\overline{Z}}{\delta x_j}\right] \tag{4}$$

$$Q_2 = \frac{\delta}{\delta x_j}\left[(D+D_t)\frac{\delta\overline{Z}^2}{\delta x_j}\right] - 2(D+D_t)\frac{\delta\overline{Z}}{\delta x_j}\frac{\delta\overline{Z}}{\delta x_j} \tag{5}$$

where $\delta/\delta x_j$ refers to numerical approximation of the derivatives and D_t denotes the eddy diffusivity. Ideally, $P_1 = P_2$ and $Q_1 = Q_2$. Since it is well known that these discrete representations do not follow the calculus of continuous variables, we at least expect small differences between the two representations when implementing the VTE. Instead, the errors associated with these approximations have a strong bias, as evidenced by the conditional means $\langle P_2|P_1\rangle$ and $\langle Q_2|Q_1\rangle$. For all three schemes considered, the amount of error is quite similar. Fig. 3(a) shows that the magnitude of P_1 is always underpredicted by representation in the form P_2. This implies that the large scale redistribution of variance is underpredicted by the VTE model, which undermines a major argument for this model's use. Turning to the Q terms, it can be seen that the conditional mean $\langle Q_2|Q_1\rangle$ lies above the diagonal, indicating that Q_2 is overpredicted. This finding holds for both a constant or dynamically modeled value of D_t; the latter case is depicted in Fig. 3(b). Higher values of Q_2 lead to higher values of $\overline{Z'}^2$ and, consequently, lower values of the variance.

These results represent errors occurring in a single evaluation of the model. In an actual simulation the VTE must be solved at each time step, allowing for an accumulation of error. In fact, the buildup of errors could be so severe that the variance predicted by the VTE approach could differ by several orders of magnitude from the true variance.

It should be noted that the variance transport equation is connected to the equation for the second moment of the scalar through the relationship

$$\frac{d\overline{Z'^2}}{dt} = \frac{d\overline{Z^2}}{dt} - \frac{d\overline{Z}^2}{dt}. \tag{6}$$

The STE model thus avoids the chain rule manipulations required to develop the equation for $\overline{Z}^2$.

A POSTERIORI RESULTS

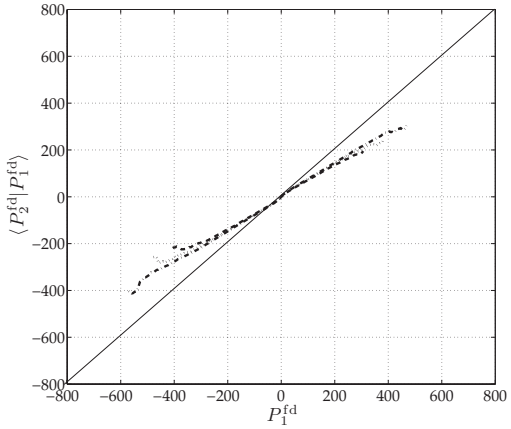
To address the importance of errors in the evolution of the filtered scalar field for subfilter scalar modeling, a novel methodology was used to conduct *a posteriori* tests. A pseudospectral code for simulation of homogeneous isotropic turbulence was modified to solve the governing equation for the filtered scalar field with exact and modified wavenumbers (Kravchenko and Moin, 1997). A second order central, fourth order central, and a sixth order central Padé scheme were considered for the approximation of first and second order derivatives in the convection and diffusion operators. A ratio of filter width to grid spacing of one is used throughout. A DNS velocity field was filtered at each time step to supply the scalar convective velocity. Models for the eddy diffusivity (Moin et al., 1991) and variance (Balarac et al., 2008) were computed with the same scheme used to evolve the filtered scalar. Because of the differences in their evolution, each scalar field constitutes a separate realization and only the statistical properties of the scalar fields should be compared.

The accuracy of the diffusion operator was found to be a critical factor in the prediction of the variance using the modified dynamic model. The filtered scalar transport equation is frequently solved in the form

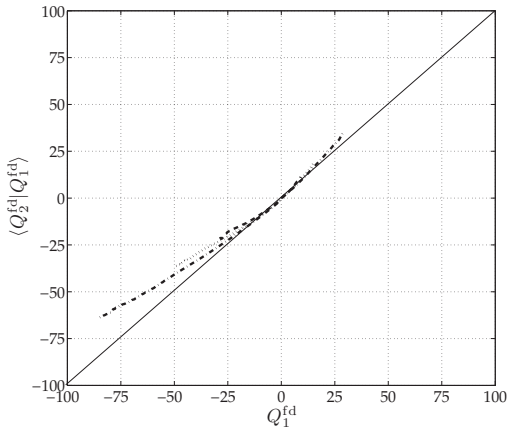
$$\frac{\partial\overline{Z}}{\partial t} + \overline{u_i}\frac{\partial\overline{Z}}{\partial x_i} = \frac{\partial}{\partial x_i}\left[(D+D_t)\frac{\partial\overline{Z}}{\partial x_i}\right] \tag{7}$$

which will be called the conventional formulation of the equation.

However, as shown in Figure 4, second derivative terms are approximated more accurately by a single application of a second derivative scheme than by two applications of a



(a) $\langle P_2|P_1\rangle$



(b) $\langle Q_2|Q_1\rangle$

Figure 3: Conditional means of variance transport terms, computed at a filter width of 32η using a variety of numerical schemes: (———) spectral (– – – –) CD-2 (· · · · · · ·) CD-4, and (— · —) P-6.

first derivative scheme. This suggests that Equation 7 be written in a modified formulation as

$$\frac{\partial \overline{Z}}{\partial t} + \overline{u_i}\frac{\partial \overline{Z}}{\partial x_i} = \frac{\partial D_t}{\partial x_i}\frac{\partial \overline{Z}}{\partial x_i} + (D + D_t)\frac{\partial^2 \overline{Z}}{\partial x_i^2} \qquad (8)$$

For comparison, a simulation was performed using an exact treatment of the diffusive terms with finite difference evaluation of the convective term. Fig. 5 compares the evolution of the filtered scalar spectra for the three cases. The choice of numerical method is relatively less consequential for the large scales of the filtered scalar field, while the effect on scales near the filter cut-off can be dramatic. Scalar evolution using Eq. 8 agrees much better with evolution using a spectrally accurate diffusive term. Inadequate diffusion allows an accumulation of energy at the small resolved scales, with a two-fold effect on the variance model.

First, the true values of the quantity $\nabla\overline{Z}\cdot\nabla\overline{Z}$ are increased. Note that the variance model is based on this gradient term (Eq. 1). In the case of the conventional formulation, the increase is great enough to remain significant when $\nabla\overline{Z}\cdot\nabla\overline{Z}$ is evaluated with finite difference methods and

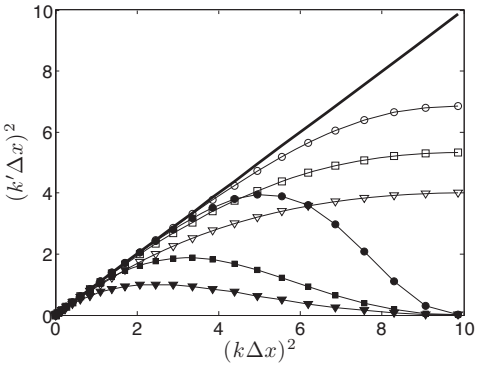


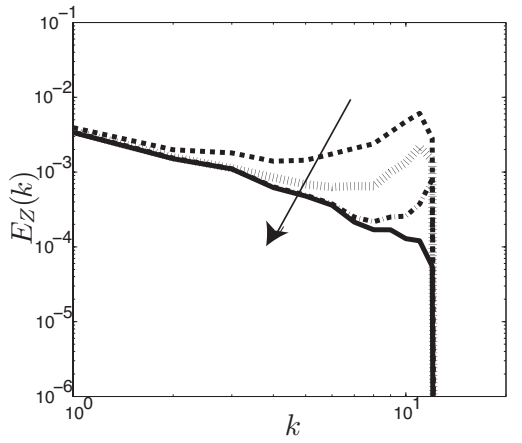
Figure 4: Modified wave numbers for single second derivative operator (open symbols) and two applications of a first derivative operator (filled symbols) for ▽ CD-2 □ CD-4, and ◯ P-6 schemes

its value is greatest for the second order scheme, followed by fourth order, sixth order, and spectral schemes. However, for the modified formulation the difference is not so strong, and there is not a consistent ordering of the schemes in terms of which predicts the highest values for the quantity. Second, the value of the model coefficient increases due to higher values of the Leonard term. For the conventional formulation, the increase in the Leonard term more than compensates for increases in the gradient term of the model closure, as shown in Fig. 6. These two factors combine for the scalar fields evolved with Eq. 7 to predict markedly higher values of the variance for lower order schemes. In Fig. 7(a) the mode of the variance distribution computed with second order methods is over an order of magnitude larger than the mode of the spectral-accuracy variance distribution, and even the sixth order scheme is in poor agreement. Lower order approaches still predict higher variance values for the scalar fields evolved with Eq. 8 but because the disparity in the gradient predictions and coefficient values is less, the differences between the variance values are smaller. In particular, Fig. 7(b) shows that there is good agreement between the predictions of the spectral and sixth order Padé methods. Still closer correspondence in the results for all schemes is achieved by the exact diffusion operator case (Fig. 7(c)).

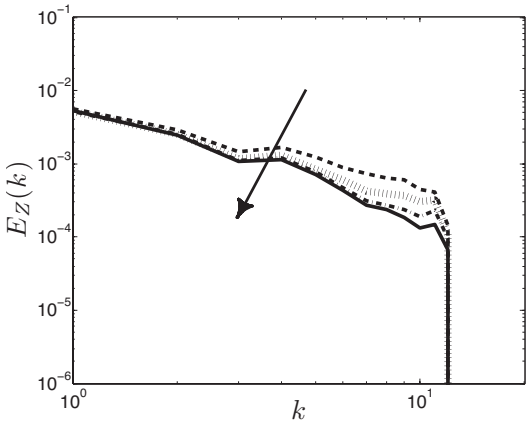
Clearly, implementations of the diffusion operator that remain effective at all wavenumbers, such as the expanded formulation considered here, help to reduce inconsistencies in variance prediction due to numerical errors. However, it must be noted that some excess scalar energy serves to offset numerical errors that occur in evaluating the dynamic model. In simulations, it is common to use discretizations of the convective term which introduce additional dissipation. This practice could, potentially, degrade the over-all accuracy of the variance model by removing too much energy.

CONCLUSIONS

The results of *a priori* and *a posteriori* analyses show that numerical error can have first-order effects on variance modeling. In many cases, the use of higher-order finite dif-



(a)



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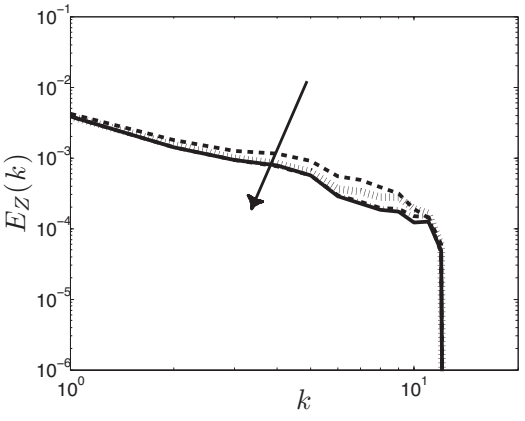
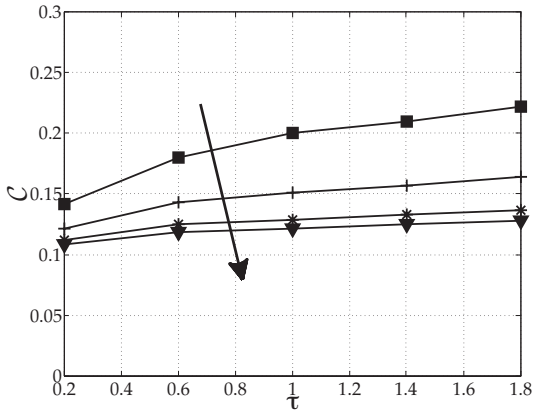
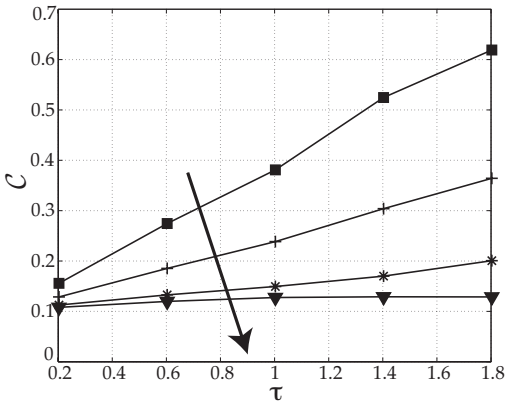


(c)

Figure 5: Filtered scalar ($\overline{Z}$) spectra at normalized time $\tau = 1.4$ using (a) Eq. 7, (b) Eq. 8, and (c) exactly calculated diffusion. Schemes shown are (– – – –) CD-2, (⋯⋯⋯) CD-4, (—·—) P-6, and (———) spectral.



(a)

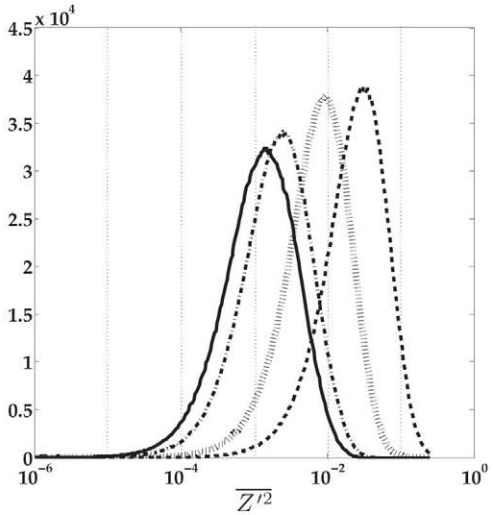


(b)

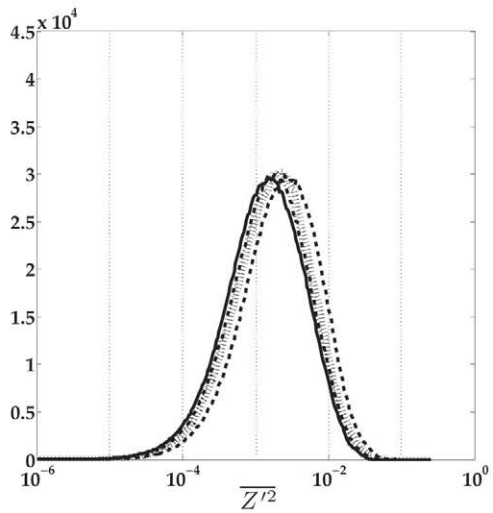
Figure 6: Evolution of model coefficient as a function of normalized time for (*a posteriori* analysis using (a) Eq. 7 and (b) Eq. 8 . Arrow indicates increasing accuracy of scheme: CD-2, CD-4, P-6, and spectral.

ference schemes produces relatively minor improvements in modeling accuracy. However, certain choices of model implementation can reduce error with little or no increase in computational effort. The accuracy of model predictions is contingent on the accuracy of the filtered scalar field from which the model is calculated. The smallest scales of the filtered field, which are critical to the prediction of the dynamic model coefficient, are sensitive to errors in the diffusion operator. The accuracy of the evolution of these scales can be increased by solving the scalar transport equation in the form of Eq. 8.

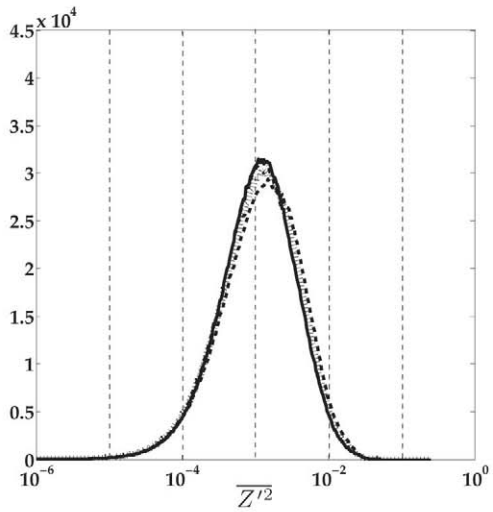
Given a filtered scalar field, finite difference methods underpredict the quantity $\nabla\overline{Z} \cdot \nabla\overline{Z}$ in the algebraic dynamic model for the variance. The underprediction of that term is partially canceled by overprediction of the dynamic coefficient, again due to underprediction of gradients. The error of the modified dynamic model (Balarac et al., 2008), unlike that of the original dynamic model (Pierce and Moin, 1998), is consistently reduced by increasing the order of accuracy of the scheme used to calculate the model, suggesting its use in



(a)



(b)



(c)

Figure 7: Distributions of $\overline{Z'^2}$ at normalized time $\tau = 1.4$ for (*a posteriori* analysis using (a) Eq. 7, (b) Eq. 8, and (c) exact diffusion operator for all scalars. Schemes shown are (– – – –)CD-2, (· · · · · · ·) CD-4, (— · —) P-6 and (————) spectral.

simulations. In the category of transport equation models, the equation for the second moment of the scalar is numerically superior to the variance transport equation, which is biased towards underprediction of the variance.

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