5A.3 SUBFILTER-SCALE SCALAR TRANSPORT FOR LARGE-EDDY SIMULATION

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1. INTRODUCTION

Large-eddy simulation (LES) is an important tool for studying meso-scale atmospheric flow fields, where practical grid sizes are much larger than what is required to resolve all of the turbulent motions. The quality of the subfilter-scale (SFS) model used to represent the unresolved motions is thus very important for accurate calculations. Cederwall and Street (1999) showed that use of an improved SFS model revealed turbulent episodes known to occur in the stable boundary layer that were not found in previous simulations.

The transport of pollutants or suspended matter is difficult to model but is of particular interest in the atmospheric boundary layer (ABL). Most simulations use an eddy diffusivity model in which the SFS transport terms are aligned with the resolved-scale strain rate and are dissipative. Here, a series expansion model is proposed for the unclosed terms of the scalar transport equation, analogous to the model presented by Street (1999) and Katopodes *et al.* (2000) for the momentum equation. This model has no free parameters, is straightforward to derive, and correlates very well with direct numerical simulation (DNS) data in *a priori* tests. The model is of scale-similar form, and thus allows backscatter, or scalar flux from the small to the large scales. This is believed to be especially important when the large scales are not fully resolved in the ABL (Mason and Thomson 1992).

To model the unclosed SFS terms in the scalar transport equation, we use successive inversion of a Taylor series expansion to express the unfiltered velocity and scalar concentration in terms of their filtered (resolved) counterparts. We then derive SFS models of arbitrary order of accuracy in the filter width. Furthermore, the SFS model satisfies the evolution equations for the SFS scalar transport to the specified order of accuracy.

In this paper, we present the derivation of the new SFS model, followed by preliminary tests of the model using *a priori* tests with DNS data of sheared, stably-stratified homogeneous turbulence. We then describe the implementation of this model and future tests, and close with a summary.

2. CLOSURE MODELS FOR SCALAR TRANSPORT

The scalar transport equation is given by

$$\frac{\partial \theta}{\partial t} + u_j \frac{\partial \theta}{\partial x_j} = \kappa \frac{\partial^2 \theta}{\partial x_j \partial x_j} \qquad (1)$$

where u_j denotes the velocity, θ is the scalar variable of interest (such as concentration or temperature), and κ is its diffusivity. Repeated indices indicate summation. Applying a spatial filter to this equation, we obtain

$$\frac{\partial \overline{\theta}}{\partial t} + \overline{u}_j \frac{\partial \overline{\theta}}{\partial x_j} = \kappa \frac{\partial^2 \overline{\theta}}{\partial x_j \partial x_j} - \frac{\partial Q_j}{\partial x_j} \qquad (2)$$

where

$$Q_j = \overline{u_j \theta} - \overline{u}_j \overline{\theta} \qquad (3)$$

is the subfilter-scale scalar flux which must be modeled. The anisotropic Gaussian filter is used here, where $\Delta_x, \Delta_y, \Delta_z$ are the filter widths in each direction. Other spatially compact filters, including asymmetric filters, give comparable results, with a change in the expansion coefficients below (see Shah 1995). It is assumed that the filtering operation commutes with the spatial derivatives, which is true for a spatially homogeneous filter. Some error is introduced if this is not so (Ghosal and Moin 1995).

The traditional procedure has been to use scaling and physical arguments to model the unclosed terms in (3). A gradient diffusion form is often assumed, where the SFS scalar flux is related to gradients of the resolved quantity by

$$Q_j = -\kappa_T \frac{\partial \overline{\theta}}{\partial x_j} \ , \qquad (4)$$

where κ_T is the scalar eddy diffusivity. In LES, a common treatment is to use the Smagorinsky model (1963), which assumes

$$\kappa_T = \frac{1}{\sigma_T} (C_S \Delta)^2 (\overline{S}_{ij} \overline{S}_{ij})^{1/2} \overline{S}_{ij} \qquad (5)$$

where C_S is the Smagorinsky constant, σ_T is the turbulent Schmidt number (usually chosen to be approximately 1), and $\overline{S}_{ij}$ is the resolved scale strain rate tensor. In ABL simulations, prognostic equations are often used to determine κ_T based on the turbulent kinetic energy (TKE).

Further developments in SFS modeling for LES have led to dynamic and mixed models (see Piomelli 1999). These improved models have not been widely applied in atmospheric simulations; Cederwall and Street (1999) used a dynamic mixed model to simulate a stable boundary layer with good results.

Here, we do not use an eddy diffusivity model as above. Instead, we use a model of the scale-similarity form, and do not assume a form for the SFS flux, but seek to model the unresolved velocity and scalar fields directly. In the spirit of velocity estimation models recently introduced (Geurts 1997, Domaradzki and Saiki 1997, Stolz and Adams 1999), we follow a mathematical approach to obtain an approximate expression for the the unresolved variables and use these to calculate the SFS scalar flux.

This model has the features of not requiring calculation of extra prognostic equations and being free of any adjustable coefficients. However, with the procedure (not

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included here) of Katopodes *et al.* (2000), it can be shown that the model presented here satisfies the evolution equations for the SFS scalar flux to fourth order in the filter width. Thus, the effects of buoyancy, Coriolis forcing, pressure, advection, and diffusion are naturally included in the model and do not need special treatment. Furthermore, the model can be specified to any desired order of accuracy.

The goal of a closure model is to express the unresolved quantities in terms of the known (computable) resolved quantities; *i.e.*, we seek to write $\theta = f(\overline{\theta})$. With that aim, we introduce a multi-dimensional Taylor expansion for the scalar field at any point,

$$\begin{aligned}\theta(x'_j) &= \theta(x_j) + (x'_m - x_m)\frac{\partial\theta(x_j)}{\partial x_m} \\ &+ \frac{1}{2}(x'_m - x_m)(x'_n - x_n)\frac{\partial^2\theta(x_j)}{\partial x_m \partial x_n} + \cdots \; , \qquad (6)\end{aligned}$$

using index notation for compactness. A similar expression can be written for the velocity field.

We now apply the Gaussian filter, which eliminates all terms with odd powers of x, y, or z, due to the filter symmetry, so that

$$\begin{aligned}\overline{\theta}(x,y,z) &= \theta + \frac{\Delta_x^2}{24}\frac{\partial^2\theta}{\partial x^2} + \frac{\Delta_y^2}{24}\frac{\partial^2\theta}{\partial y^2} + \frac{\Delta_z^2}{24}\frac{\partial^2\theta}{\partial z^2} \\ &+ \frac{\Delta_x^4}{1152}\frac{\partial^4\theta}{\partial x^4} + \frac{\Delta_y^4}{1152}\frac{\partial^4\theta}{\partial y^4} + \frac{\Delta_z^4}{1152}\frac{\partial^4\theta}{\partial z^4} \\ &+ \frac{\Delta_x^2\Delta_y^2}{1728}\frac{\partial^4\theta}{\partial x^2\partial y^2} + \frac{\Delta_y^2\Delta_z^2}{1728}\frac{\partial^4\theta}{\partial y^2\partial z^2} \\ &+ \frac{\Delta_x^2\Delta_z^2}{1728}\frac{\partial^4\theta}{\partial x^2\partial z^2} + O(\Delta^6) \; . \qquad (7)\end{aligned}$$

Rearranging and using this expression recursively, we obtain

$$\begin{aligned}\theta(x,y,z) &= \overline{\theta} - \frac{\Delta_x^2}{24}\frac{\partial^2\overline{\theta}}{\partial x^2} - \frac{\Delta_y^2}{24}\frac{\partial^2\overline{\theta}}{\partial y^2} - \frac{\Delta_z^2}{24}\frac{\partial^2\overline{\theta}}{\partial z^2} \\ &+ \frac{\Delta_x^4}{1152}\frac{\partial^4\overline{\theta}}{\partial x^4} + \frac{\Delta_y^4}{1152}\frac{\partial^4\overline{\theta}}{\partial y^4} + \frac{\Delta_z^4}{1152}\frac{\partial^4\overline{\theta}}{\partial z^4} \\ &+ \frac{5\Delta_x^2\Delta_y^2}{1728}\frac{\partial^4\overline{\theta}}{\partial x^2\partial y^2} + \frac{5\Delta_y^2\Delta_z^2}{1728}\frac{\partial^4\overline{\theta}}{\partial y^2\partial z^2} \\ &+ \frac{5\Delta_x^2\Delta_z^2}{1728}\frac{\partial^4\overline{\theta}}{\partial x^2\partial z^2} + O(\Delta^6) \; , \qquad (8)\end{aligned}$$

which expresses the full scalar at a point (x, y, z) in terms of the filtered scalar at that point. If the filter is isotropic, (8) reduces to

$$\begin{aligned}\theta &= \overline{\theta} - \frac{\Delta^2}{24}\nabla^2\overline{\theta}_i + \frac{\Delta^4}{1152}\left(\frac{\partial^4\overline{\theta}}{\partial x^4} + \frac{\partial^4\overline{\theta}}{\partial y^4} + \frac{\partial^4\overline{\theta}}{\partial z^4}\right) \\ &+ \frac{5\Delta^4}{1728}\left(\frac{\partial^4\overline{\theta}}{\partial x^2\partial y^2} + \frac{\partial^4\overline{\theta}}{\partial y^2\partial z^2} + \frac{\partial^4\overline{\theta}}{\partial x^2\partial z^2}\right) + O(\Delta^6) \; . \qquad (9)\end{aligned}$$

This simplified form of the expansion will be used in the remaining derivations, as the anisotropic form is more cumbersome algebraically. Terms of $O(\Delta^4)$ and higher will also be ignored subsequently. The anisotropic results to fourth order can be recovered by replacing $\frac{\Delta^2}{24}\nabla^2$ by

$$\frac{\Delta_x^2}{24}\frac{\partial^2}{\partial x^2} + \frac{\Delta_y^2}{24}\frac{\partial^2}{\partial y^2} + \frac{\Delta_z^2}{24}\frac{\partial^2}{\partial z^2} \; . \qquad (10)$$

Now we can derive models for Q_j by substituting the series expansions for θ (9) and the analogous expression for velocity directly into (3). When both the unclosed and explicit terms are expanded, and terms fourth order and higher are neglected, we obtain

$$\begin{aligned}Q_j &= \overline{\overline{u}_i\overline{\theta}} - \overline{\overline{u}}_i\overline{\overline{\theta}} - \frac{\Delta^2}{24}\overline{\overline{u}_i\nabla^2\overline{\theta}} - \frac{\Delta^2}{24}\overline{\overline{\theta}\nabla^2\overline{u}_i} \\ &+ \frac{\Delta^2}{24}\overline{\overline{u}}_i\nabla^2\overline{\overline{\theta}} + \frac{\Delta^2}{24}\overline{\overline{\theta}}\nabla^2\overline{\overline{u}}_i + O(\Delta^6) \; . \qquad (11)\end{aligned}$$

The first two terms are analogous to the Leonard terms in the SFS stress; the higher order derivative terms can be shown to be dissipative (Clark 1977).

3. A PRIORI TESTS

A priori tests for several SFS models are performed using a direct numerical simulation (DNS) dataset for stably-stratified homogeneous shear flow computed by Shih *et al.* (2000). *A priori* tests indicate the degree of correlation between the modeled and exact subfilter-scale terms (see Clark 1977). They are useful indications of the expected performance of a SFS model in actual LES computations (*a posteriori* tests), even though in this case the DNS data is for low Reynolds number flow. The DNS data are sampled on the scale of the LES grid and filtered using an anisotropic Gaussian filter to obtain the LES field, $\overline{u}_i$. Then the LES field can be used to generate higher order approximations using variations of (11).

Tables 1-2 show correlation coefficients (C) and ratios (R) for the subfilter-scale quantities: Q_i is the SFS flux, $\partial Q_j/\partial x_j$ is the divergence of the subfilter flux which appears in the transport equations, and $Q_j\partial\overline{\theta}/\partial x_j$ is the SFS scalar dissipation. The ratio is the exact DNS rms value divided by the modeled rms value, and should be close to one. For the scalar dissipation term, the ratio gives an indication of the magnitude of the scalar dissipation which is captured by the model. For comparison, the equivalent momentum terms are also listed.

Results are presented for the Smagorinsky (S), and 2nd- (E2), 4th- (E4), and 6th-order (E6) series expansion models (using (11)). Several other models were tested, but results are not presented here. The E2 model is of the scale-similar form considered by Bardina *et al.* (1983) for the SFS stress. LES to DNS grid ratios of $GR = 2, 4, 8$ are considered, where $\Delta_{LES} = GR\ \Delta_{DNS}$. (Only the $GR = 2, 8$ cases are shown here.) In each case the filter-grid ratio is $FGR = \Delta/\Delta_{LES} = 2$.

For the E6 model and $GR = 2$, the correlation for the SFS scalar dissipation is 0.999, with the ratio of rms exact to modeled values at 1.021, indicating that the SFS dissipation is captured to within 2%. On the other hand, the Smagorinsky model for this case exhibits a correlation of -0.010, and a ratio of 1.904, indicating that the representation of the SFS motions is extremely poor. In mesoscale simulations of the atmosphere, the grid size will be considerably larger than the DNS grid size, making it harder to accurately construct the SFS motions using the knowledge of the resolved scales only. However, even for $GR = 8$, the E6 model gives a ratio for the SFS scalar dissipation of 1.273, with a correlation much higher than any other model tested, at 0.973.

To illustrate the performance of the series model in representing the unresolved field, Figure 1 shows contours of the scalar field with different levels of approximation for θ, as given by (8). The raw DNS data, which is sampled on an LES grid defined by $GR = 8$, is best represented by the 6th-order model; contours shown for this case (Fig. 1d) indicate that the smaller features of the DNS data (Fig. 1a) are captured quite well, unlike the lower order models.

4. IMPLEMENTATION

As we have formulated a closed expression for Q_j as given in (11), this can be directly substituted into the resolved flow equation, (2), which can then be discretized and solved numerically. Using this series closure model thus eliminates the need for prognostic equations for quantities such as turbulent kinetic energy that are usually used for turbulence closure in atmospheric models. Furthermore, there are no parameters which need to be adjusted or calculated (*cf.* the standard TKE models or dynamic Smagorinsky or dynamic mixed closure models). The model should therefore not be computationally intensive.

No assumptions about the discretization were made in any of the derivations above. However, it is important that the filter width be at least twice the size of the grid spacing. Otherwise, as shown by Ghosal (1996), discretization error will be as large as the effect of the SFS model.

The greatest challenge in implementing this model will be applying the necessary filtering and calculating higher order derivatives near solid boundaries. This issue is under investigation.

5. CONCLUSION

The series model is easy to implement and provides an estimate of the SFS flux to any order of accuracy desired. While the model will be tested further in actual LES (*a posteriori* tests) of the atmosphere, the *a priori* tests presented here indicate that the series expansion model is considerably better than the eddy diffusivity closure models traditionally used to represent SFS scalar transport. The model has no free parameters and does not require the solution of additional prognostic equations. The series model satisfies the evolution equations for the SFS flux to the appropriately predefined order of accuracy, meaning that it is influenced by buoyancy, Coriolis, pressure, advection, and diffusion effects. It is expected that an improved SFS closure model will lead to significantly more accurate simulations of the atmospheric boundary layer, yielding insight into turbulent motions which transport pollutants..

5. ACKNOWLEDGMENTS

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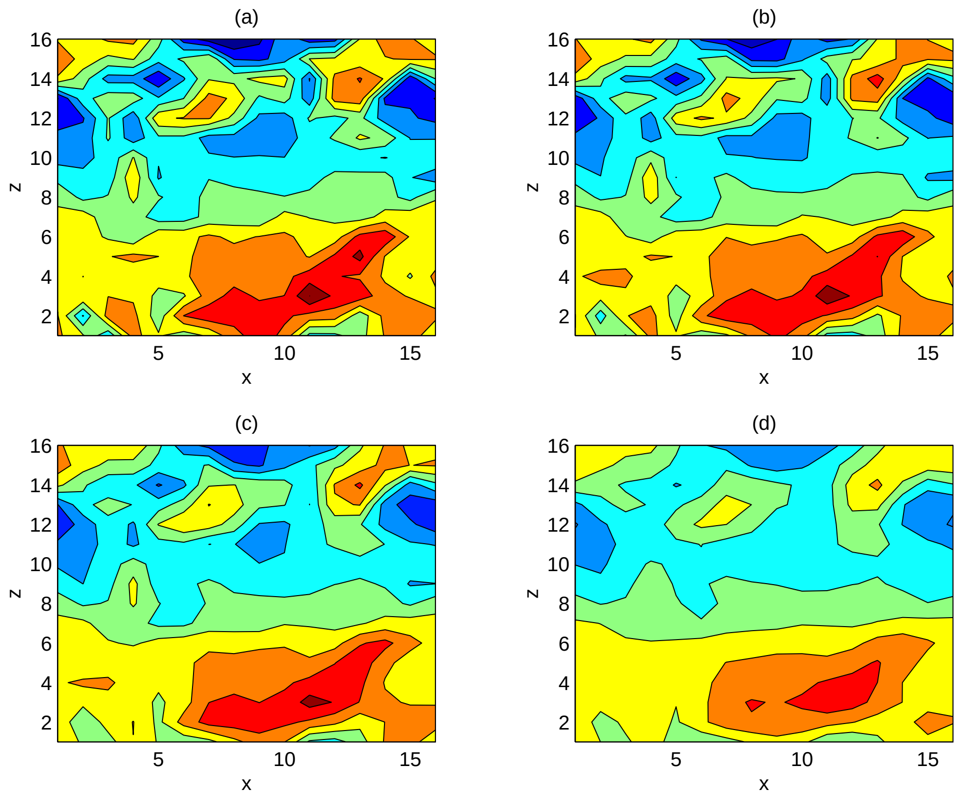

Figure 1: Contour plots of LES estimates for θ on an x_1, x_3-plane, $GR = 8$. (a) Sampled DNS field; (b) 6th-order estimate; (c) 4th-order estimate; (d) 2nd-order estimate.

		τ_{12}	$\frac{\partial \tau_{1j}}{\partial x_j}$	$\tau_{ij}\frac{\partial u_i}{\partial x_j}$	Q_1	Q_2	Q_3	$\frac{\partial Q_j}{\partial x_j}$	$Q_j\frac{\partial \overline{\rho}}{\partial x_j}$
S	C	0.1610	0.4746	0.6962	−0.1678	−0.0098	0.0094	0.0019	−0.0097
	R	3.5042	2.8092	1.4780	3.6150	0.6964	1.1373	0.4328	1.9040
$E2$	C	0.9525	0.9194	0.9665	0.9697	0.9354	0.9451	0.9196	0.9876
	R	1.3367	1.9179	1.3666	1.4497	1.4200	1.4629	2.0252	1.4350
$E4$	C	0.9875	0.9763	0.9917	0.9921	0.9803	0.9851	0.9739	0.9973
	R	1.0702	1.2636	1.0724	1.1242	1.0933	1.1085	1.2968	1.1032
$E6$	C	0.9969	0.9937	0.9972	0.9980	0.9941	0.9959	0.9916	0.9994
	R	1.0097	1.0611	1.0062	1.0346	1.0160	1.0209	1.0750	1.0207

Table 1: Gaussian Filter: Correlations, $GR = 2$, $FGR = 2$.

		τ_{12}	$\frac{\partial \tau_{1j}}{\partial x_j}$	$\tau_{ij}\frac{\partial u_i}{\partial x_j}$	Q_1	Q_2	Q_3	$\frac{\partial Q_j}{\partial x_j}$	$Q_j\frac{\partial \overline{\rho}}{\partial x_j}$
S	C	0.0925	0.3041	0.3920	−0.2494	0.0064	0.0842	0.0148	−0.0395
	R	4.9880	3.1754	2.0092	11.7193	1.8005	2.7365	1.3796	2.8186
$E2$	C	0.7759	0.7852	0.8181	0.8901	0.7516	0.7583	0.7857	0.9047
	R	2.8324	4.1177	3.1285	2.7467	2.8250	2.9520	4.5566	2.8349
$E4$	C	0.8769	0.8729	0.8939	0.9431	0.8553	0.8595	0.8684	0.9459
	R	1.5989	2.0326	1.7325	1.5968	1.6290	1.6734	2.2085	1.6354
$E6$	C	0.9407	0.9326	0.9422	0.9733	0.9231	0.9288	0.9284	0.9727
	R	1.2301	1.4111	1.3038	1.2506	1.2676	1.2895	1.5104	1.2727

Table 2: Gaussian Filter: Correlations, $GR = 8$, $FGR = 2$.