Toward Numerical Modeling in the “Terra Incognita”

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ABSTRACT

In mesoscale modeling the scale \( l \) of the energy- and flux-containing turbulence is much smaller than the scale \( \Delta \) of the spatial filter used on the equations of motion, and in large-eddy simulation (LES) it is much larger. Since their models of the subfilter-scale (SFS) turbulence were not designed to be used when \( l \) and \( \Delta \) are of the same order, this numerical region can be called the “terra incognita.”

The most common SFS model, a scalar eddy diffusivity acting on the filtered fields, emerges from the conservation equations for SFS fluxes when several terms, including all but one of the production terms, are neglected. Analysis of data from the recent Horizontal Array Turbulence Study (HATS) shows that the neglected production terms can be significant. Including them in the modeled SFS flux equations yields a more general SFS model, one with a tensor rather than a scalar eddy diffusivity. This more general SFS model is probably not necessary in fine-resolution LES or in coarse-resolution mesoscale modeling, but it could improve model performance in the terra incognita.

1. Introduction

The numerical modeling of turbulent flows has advanced steadily since the advent of the large-scale digital computer in the 1960s. In smaller-scale meteorological applications today (domain sizes from 3000 to 1 km, say) one can identify two broad classes of such modeling: mesoscale modeling on the larger domains and large-eddy simulation (LES) on the smaller ones. Their fundamental difference is the value of \( l/\Delta \), the ratio of the energy-containing turbulence scale and the scale of the spatial filter used on the equations of motion. In traditional mesoscale modeling \( l/\Delta \) is small, so none of the turbulence is resolved; in traditional LES it is large, so the energy- and flux-containing turbulence is resolved.

Until recently the \( l/\Delta \) values and spatial domains of mesoscale modeling and LES were nonoverlapping; the horizontal area of a typical boundary layer LES domain could fit within the horizontal grid mesh square of a typical mesoscale model. Today’s computers allow as many as \( 10^6 \) numerical grid points in dynamical models (Gotoh and Fukayama 2001), so it is now possible to do very-fine-mesh mesoscale modeling with \( l/\Delta \sim 1 \). This is approaching the \( l/\Delta \) range traditionally used in the relatively coarse-resolution LES of severe storms. Since neither LES nor mesoscale modeling was designed to operate in this \( l/\Delta \) range, we shall term it the “terra incognita.”

2. Three-dimensional simulation of turbulent flow

a. The foundations

Numerical simulation of high-Reynolds-number turbulent flows is possible only after the equations of motion have been spatially smoothed to remove the fine structure of their solution fields. Lilly’s (1967) derivations of the smoothed equations and the equation for the Reynolds stress that results provided the basis of what is known today as large-eddy simulation, or LES.

Lilly smoothed the flow variables by averaging them over a cube of side \( h \), denoting the averaging by an overbar:

\[
\bar{F}(x, t) = \frac{1}{h^3} \int_{-h/2}^{h/2} \int_{-h/2}^{h/2} \int_{-h/2}^{h/2} F(x + x', t) \, dx'_1 \, dx'_2 \, dx'_3.
\]

(1)

We shall adopt Leonard’s (1974) generalization to spatial filtering,

\[
\bar{F}(x, t) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} F(x + x', t) G(x - x') \, dx'_1 \, dx'_2 \, dx'_3,
\]

(2)

with \( \bar{F} \) a filtered variable and \( G \) the filter function. Following today’s convention we shall designate the spatial scale of the filter function as \( \Delta \).
The Navier–Stokes and continuity equations for constant-density flow are

$$\frac{\partial u_i}{\partial t} + \frac{\partial u_i u_j}{\partial x_j} = -\frac{\partial (\rho p)}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j \partial x_j} \frac{\partial u_i}{\partial x_j} = 0. \quad (3)$$

Filtering these equations produces

$$\frac{\partial \overline{u_i}}{\partial t} + \frac{\partial \overline{u_i u_j}}{\partial x_j} = -\frac{\partial (\overline{\rho p})}{\partial x_i} + \nu \frac{\partial^2 \overline{u_i}}{\partial x_j \partial x_j},$$

$$\frac{\partial \overline{u_i}}{\partial x_i} = 0; \quad (4)$$

$$\tau_{ij}$$ is a deviatoric (meaning its isotropic value has been subtracted) kinematic Reynolds stress defined as

$$\tau_{ij} = -(\overline{u_i u_j} - \overline{u_i}\overline{u_j}) + \frac{2}{3}\delta_{ij}e = -\left(R_{ij} - \frac{2}{3}\delta_{ij}e\right). \quad (5)$$

The second term on the left is advection by the filtered velocity; the third term is the divergence of a flux due to SFS motions. The first two terms on the right are rates of production, the first due to interaction of SFS motions that have been removed by the filtering,

$$e = (\overline{\tau_{ij}} - \overline{\tau_{ij}})/2. \quad (6)$$

Moreover, $$\tau_{ij}$$ has zero trace (i.e., $$\tau_{ii} = 0$$), which aids its modeling. We shall call $$\tau_{ij}$$ simply the subfilter-scale (SFS) stress and $$e$$ the SFS energy.

The first pressure term is presumably a destruction rate since the molecular-destruction term has vanished under the assumption of local isotropy; the second pressure term is modeling its pressure-destruction term as

$$\frac{\partial \tau_{ij}}{\partial t} = u_i \frac{\partial \tau_{ij}}{\partial x_i} + u_j \frac{\partial \tau_{ij}}{\partial x_j} - \left(\overline{\tau_{ij}} - \frac{2}{3}\delta_{ij}e\right), \quad (7)$$

which indicates how the evolution equation for $$\tau_{ij}$$ is derived. With the assumption of local isotropy its viscous dissipation term vanishes and Lilly’s $$\tau_{ij}$$ equation reduces to

$$\tau_{ij} = K \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i}\right) = KD_{ij}, \quad (9)$$

with $$e$$ the kinetic energy per unit mass of the small-scale motions that have been removed by the filtering,

$$E(\kappa) = \alpha e^{3/4} \sim^{3/4}. \quad (11)$$

Lilly (1966) showed that this implies

$$k = 0.23 \alpha^{-3/4}. \quad (12)$$

Lilly’s scalar-eddy-viscosity model (9) can be interpreted as arising from his $$\tau_{ij}$$ conservation equation (8) under two simplifications. The first is the neglect of its time-change, advection, flux-divergence, and second production term. The second is modeling its pressure-destruction term as $$-\tau_{ij}/T$$, with $$T$$ a time scale; this is the simplest model that ensures its being a sink. In this limit (8) becomes a two-term balance that yields Lilly’s closure (9),

$$\tau_{ij} = 2eTD_{ij} = KD_{ij}. \quad (13)$$

It is not clear how to justify the neglect of the second production term in (8), however. We shall see that retaining this term (and its counterpart in the SFS scalar flux conservation equation) yields a more general closure, one implying an eddy diffusivity that is a tensor quantity rather than a scalar.

b. The mesoscale and LES limits of the filtered equations

Lilly’s evolution equation (8) for SFS stress holds for any averaging that commutes with differentiation. That
includes not only spatial averaging and its generalization by Leonard (1974) to spatial filtering, but also the ensemble averaging of classical turbulence analysis. In an unbounded, homogeneous field low-pass spatial filtering converges to ensemble averaging as $\Delta \to \infty$. (In a flow that is homogeneous in the horizontal but not the vertical, we restrict the averaging to the horizontal plane.) Thus, we can explore both types of averaging by allowing the filter scale $\Delta$ to vary, subject only to the restriction that it be much larger than the scale of the dissipative eddies so that the molecular-diffusion terms in the filtered equations are negligible.

We shall call the case $l \gg \Delta$, with $l$ the integral scale of the turbulence, the “LES limit.” Here the energy and flux-containing turbulence is contained in the filtered equation of motion (4), as sketched in Fig. 1. The “mesoscale limit” $l \ll \Delta$ is reached in mesoscale modeling. [Adding a Coriolis term to Eq. (4) presents no complications, since that term is linear in velocity, so we shall not indicate it explicitly. In general, there is also a buoyancy term, but it does not change the central issues, and we shall neglect it as well.] In mesoscale modeling the grid-mesh element is typically much smaller in the vertical direction than in the horizontal in order to resolve some structure in the boundary layer. But, since resolving three-dimensional turbulence requires a grid mesh that is smaller than $l$ in all three directions, even with fine vertical resolution essentially none of the turbulence is resolved in the mesoscale limit. The turbulence resides in the SFS fields, as also sketched in spectral terms in Fig. 1.

Equation (8) is the evolution equation for the SFS stress $\tau_{ij}$ in LES, in mesoscale modeling, and for applications over the range of scales in between. Even though in high-resolution LES the turbulent kinetic energy and fluxes are carried almost entirely by the filtered motion, the $\tau_{ij}$ term in (4) remains important. It is essential to the transfer of kinetic energy and scalar variance from the filtered to subfilter scales (Wyngaard 2002). Thus, reliable models of $\tau_{ij}$ and $e$ are required also in the LES limit.

3. The flux conservation equations as guides for SFS modeling

a. A conserved scalar

The evolution equation for a conserved scalar $c$ in a constant-density flow is

$$\frac{\partial c}{\partial t} + u_i \frac{\partial c}{\partial x_i} = \gamma \frac{\partial^2 c}{\partial x_i \partial x_j}. \quad (14)$$

The filtered equation is

$$\frac{\partial \bar{\sigma}^2}{\partial t} + \bar{\nu}_i \frac{\partial \bar{\sigma}^2}{\partial x_i} + \frac{\partial (2f \bar{\sigma})}{\partial x_i} = 2f_i \frac{\partial \bar{\sigma}}{\partial x_i}. \quad (15)$$

since $\Delta$ has been assumed large enough to make the molecular diffusion terms negligible. We shall call $f_i$ the SFS flux of the scalar.

Multiplying Eq. (15) by $2\bar{\sigma}$ and rearranging yields the equation for the evolution of the squared filtered scalar:

$$\frac{\partial \bar{\sigma}^2}{\partial t} + \bar{\nu}_i \frac{\partial \bar{\sigma}^2}{\partial x_i} + \frac{\partial (2f \bar{\sigma})}{\partial x_i} = 2f_i \frac{\partial \bar{\sigma}}{\partial x_i}. \quad (16)$$

The equation for the squared SFS scalar is

$$\frac{\partial (c^2 - \bar{c}^2)}{\partial t} + \bar{\nu}_i \frac{\partial (c^2 - \bar{c}^2)}{\partial x_i} + \frac{\partial (u_i c - \bar{\nu}_i \bar{c}^2 - 2f \bar{\sigma})}{\partial x_i} = -2\chi - 2f_i \frac{\partial \bar{\sigma}}{\partial x_i}. \quad (17)$$

with $2\chi$ the rate of destruction of $\bar{c}^2$ through molecular diffusion. Evidently the final term in (17) is the rate of gain of squared scalar through transfer from the filtered field; it appears as a rate of loss in (16).

Wyngaard et al. (1971) and Deardorff (1973) have discussed the evolution equation for $f_i$. In a constant-density flow it can be written as

$$\frac{\partial f_i}{\partial t} + \bar{u}_i \frac{\partial f_i}{\partial x_i} + \bar{\nu}_j \frac{\partial f_i}{\partial x_j} + \frac{\partial}{\partial x_j} (u_j u_i - \bar{u}_j \bar{u}_i - \bar{\nu}_j \bar{u}_i - \bar{\nu}_i \bar{u}_j + 2\bar{\sigma} \bar{u}_i u_j) = -f_i \frac{\partial \bar{\nu}_i}{\partial x_j} - R_{ij} \frac{\partial \bar{\sigma}}{\partial x_j} - \frac{\partial}{\partial x_j} (\bar{p} \bar{u}_i - \bar{p} \bar{u}_i) + \left( \frac{\partial c}{\partial x_j} - \frac{\partial \bar{c}}{\partial x_j} \right). \quad (18)$$
The second term on the left is the advection of \( f_i \) by the filtered velocity; the third term is the divergence of the SFS flux of \( f_i \). The first term on the right is the rate of production of \( f_i \) through the amplification and rotation of scalar flux by the filtered velocity gradient; it is the counterpart of the “stretching and tilting” term in the vorticity equation. The second term on the right represents the rate of production through the interaction of an SFS stress and the filtered scalar gradient. The third term is the gradient of a pressure covariance, and the final term represents the interaction of pressure and \( c \) gradients. The neglected molecular term is quite small in large Reynolds number turbulence (Wyngaard et al. 1971).

The second and third terms on the left side and the third term on the right side of (18) simply move \( f_i \) around in space, and the first two terms on the right are source terms. Thus, the role of principal sink for scalar flux falls to the pressure, \( c \)-gradient term. The simplest model for it is \(-f_i/T_c\), with \( T \) a time scale of the SFS turbulence. Making all but one of the assumptions that Lilly used to simplify Eq. (8) for \( \tau_{ij} \)—that is, dropping the time-change, advection, and flux-divergence terms but retaining all the production terms—yields the closure

\[
f_i = -T \left( \frac{\partial \sigma}{\partial x_i} + R_{ij} \frac{\partial \sigma}{\partial x_j} \right). \tag{19}
\]

This implies the six-term model for SFS flux

\[
f_i = -T \left( f_{i1} \frac{\partial \sigma}{\partial x_1} + f_{i2} \frac{\partial \sigma}{\partial x_2} + f_{i3} \frac{\partial \sigma}{\partial x_3} + R_{ij} \frac{\partial \sigma}{\partial x_j} + R_{ij} \frac{\partial \sigma}{\partial x_j} + R_{ij} \frac{\partial \sigma}{\partial x_j} \right). \tag{20}
\]

This reduces to the usual gradient-diffusion model only if all production terms except the one involving the scalar gradient in the direction of the flux are dropped. In this limit it yields

\[
f_a = -TR_{aa} \frac{\partial \sigma}{\partial x_a} = -K \frac{\partial \sigma}{\partial x_a}, \quad \text{no sum on } \alpha. \tag{21}
\]

We shall call the production term that yields (21) the gradient-diffusion term.

In the mesoscale limit \( l \ll \Delta \), we can interpret the overbar as an ensemble average, which we shall denote by angle brackets. Then with the classical decomposition into ensemble-mean plus fluctuating parts, \( c = \langle c \rangle + c', \ u_i = \langle u_i \rangle + u'_i = U_i + u'_i \), we have \( f_i = \langle c' u'_j \rangle, \ R_{ij} = \langle u'_i u'_j \rangle \) and Eq. (19) becomes

\[
\langle c' u' \rangle = -T \left( \langle c' u'_j \rangle \frac{\partial U_j}{\partial x_i} + \langle u'_i u'_j \rangle \frac{\partial c}{\partial x_j} \right). \tag{22}
\]

Wyngaard et al. (1971) found the model (22) to be a good representation of both horizontal and vertical components of the near-neutral, ensemble-average potential temperature flux budget in the surface layer if \( T \sim Il^{-1/2} \), a time scale of the energy-containing turbulence. The horizontal flux \( \langle c' u'_j \rangle \), whose magnitude can be larger than that of the vertical flux in the surface layer, exists in the absence of a horizontal mean temperature gradient. As we shall show shortly, this implies that the eddy diffusivity for potential temperature is a tensor, not a scalar.

In the LES limit \( l \gg \Delta \) the time scale \( T \) is of the order of \( \Delta e^{1/2} \), a time scale of inertial-range turbulence. In LES practice only the gradient-diffusion contribution to Eq. (19) is typically retained, however. Deardorff (1973) rationalized this by assuming the isotropic forms \( f_i = 0, R_{ij} = 2e \delta_{ij} / 3 \) on the right side of Eq. (19), thereby eliminating all but the gradient-diffusion term and yielding Eq. (21) with \( K \sim e^{1/2} \Delta \). With this standard eddy-diffusivity model for \( f_i \), the rate of transfer of squared scalar from filtered to SFS scales, the last term in Eq. (17), is positive definite:

\[
-2f \frac{\partial \sigma}{\partial x_i} = 2K \frac{\partial \sigma}{\partial x_i} \frac{\partial c}{\partial x_j} R_{ij} \tag{23}
\]

Deardorff’s assumption of isotropy is inappropriate for \( f_i \) and \( R_{ij} \) in Eq. (19) in the LES limit since these are locally averaged quantities, not ensemble means, and are not subject to the constraints of isotropy. The assumption is also inappropriate in the mesoscale limit, where \( f_i \) and \( R_{ij} \) are energy-containing-range properties and necessarily anisotropic. Thus, the simplest consistent model of SFS scalar flux that seems applicable across the scale range is Eq. (19). With that fuller model of \( f_i \), the rate of transfer of squared scalar becomes

\[
-2f \frac{\partial \sigma}{\partial x_i} = 2T \left( \frac{\partial \sigma}{\partial x_i} \frac{\partial \sigma}{\partial x_j} f_{ij} + \frac{\partial \sigma}{\partial x_i} \frac{\partial \sigma}{\partial x_j} R_{ij} \right). \tag{24}
\]

As we shall see, this allows “backscatter,” the local transfer of variance from smaller scales to larger.

The solution of Eq. (19) for \( f_i \) can be formally written as

\[
f_i = -K_{ij} \frac{\partial \sigma}{\partial x_j}, \tag{25}
\]

with \( K_{ij} \) an eddy diffusivity that depends on \( T, \frac{\partial \sigma}{\partial x_j}, \) and \( R_{ij} \). Unlike the usual eddy diffusivity, which is a scalar quantity, \( K_{ij} \) is a second-order tensor. Rather than solving Eq. (19) for \( K_{ij} \), however, it could be more convenient to carry the time-dependent form,

\[
\frac{\partial f_{ij}}{\partial t} + f_{ij} \frac{\partial \sigma}{\partial x_j} + R_{ij} \frac{\partial \sigma}{\partial x_j} = -f_{ij} \frac{T}{T_c}. \tag{26}
\]

The time scale \( T \) is of order \( Il^{-1/2} \) and \( \Delta e^{1/2} \) in the mesoscale and LES limits, respectively. Its proportionality to \( \Delta e^{1/2} \) in the LES limit can be determined in the general way laid out by Lilly (1967). Its proportionality to \( Il^{-1/2} \) away from the LES limit would probably be different in unstable and stable stratification, as is typically found in other closures.
b. Stress

The kinetic energy equation for the filtered motion is formed by multiplying Eq. (4) by \( \pi_j \) and rearranging:

\[
\frac{\partial}{\partial t} \left( \frac{\pi_i \pi_j}{2} \right) + \pi_i \frac{\partial}{\partial x_j} \left( \frac{\pi_i \pi_j}{2} \right) = - \frac{\partial}{\partial x_j} (p^* \pi_j - \pi_j \pi_j) - \frac{1}{2} \tau_{ij} D_{ij}. \tag{27}
\]

Here \( p^* = \rho \rho + 2e/3 \) is a modified kinematic pressure. The right side of (27) represents the rate of energy transfer between filtered and subfilter scales. With the eddy-diffusivity closure (9) for \( \tau_{ij} \), this energy-transfer term becomes

\[
\frac{1}{2} \tau_{ij} D_{ij} = \frac{K}{2} \Delta^2,
\]

which is positive definite, so the energy transfer is always from filtered to subfilter scales. The \( K \) closure (9) is commonly used in LES, where this one-way energy transfer is computationally advantageous. However, the equilibrium values of \( \tau_{ij} \) components implied by (9) can be unphysical in the mesoscale limit. In the neutral atmospheric surface layer, for example, (9) yields \( \langle u'^2 \rangle = \langle w'^2 \rangle = 2e/3 \), which agrees poorly with observations.

The next level of approximation for \( \tau_{ij} \) uses the quasi-steady, homogeneous form of its conservation equation (8):

\[
\frac{\partial \tau_{ij}}{\partial t} = 0 = \frac{2}{3} e D_{ij} - \left( \tau_{ij} \frac{\partial \pi_i}{\partial x_j} + \tau_{ij} \frac{\partial \pi_j}{\partial x_i} \right)
- \left[ \frac{1}{3} \delta_{ij} \tau_{kl} D_{kl} \right] - \tau_{ij} \frac{T}{T}.
\]

with \( T \) again a time scale of the SFS turbulence. This yields the closure

\[
\tau_{ij} = \frac{2}{3} e T D_{ij} - \frac{T}{T} \left( \tau_{ii} \frac{\partial \pi_i}{\partial x_j} + \tau_{ij} \frac{\partial \pi_j}{\partial x_i} \right) - \left[ \frac{1}{3} \delta_{ij} \tau_{kl} D_{kl} \right]. \tag{30}
\]

Here, again, the implied eddy diffusivity is a second-order tensor rather than a scalar.

The rate of energy transfer from the filtered to subfilter scales is now

\[
\frac{1}{2} \tau_{ij} D_{ij} = \frac{1}{3} e T D^2 - \frac{T}{2} \left( \tau_{ii} \frac{\partial \pi_i}{\partial x_j} + \tau_{ij} \frac{\partial \pi_j}{\partial x_i} \right).	ag{31}
\]

The contribution of the last term in Eq. (30) disappearing due to continuity. Equation (30) could give local backscatter. In the mesoscale limit it implies that the turbulent velocity variances in the horizontally homogenous, near-neutral surface layer are

\[
\langle u'^2 \rangle = T \left( -2 \langle u' w' \rangle \frac{\partial U}{\partial z} - \frac{2e}{3} \right) + \frac{2e}{3},
\]

\[
\langle w'^2 \rangle = \langle w'^2 \rangle = T \left( -\frac{2e}{3} \right) + \frac{2e}{3},
\]

which with the proper choice of \( T \) can be made to agree well with observations.

c. Relation to previous work

In Deardorff’s early applications of what we now call LES to turbulent channel flow (Deardorff 1970) and to the planetary boundary layer (Deardorff 1972), the SFS model was the eddy-diffusivity closure of Eq. (9) with Smagorinsky’s form, Eq. (10), for the eddy diffusivity \( K \). Computational difficulties forced him to treat the stably stratified capping inversion in the latter work as a rigid lid. In his next study he developed a new SFS model based on the SFS flux conservation equations and was able to treat the capping inversion directly (Deardorff 1973). Findikakis and Street (1979) later reduced these SFS flux conservation equations to an “algebraic model,” much as we have outlined here, specifically for application of LES to stratified flows. Schmidt and Schumann (1989) used such an algebraic SFS model in LES of the convective boundary layer.

The SFS flux conservation equations improved the simulations, Deardorff (1973) said, although they increased the computation time by about a factor of 2.5. He used them also in his simulations of the Wangara boundary layer experiment (Deardorff 1974a,b). But later, in simulating cloudy boundary layers, he returned to the \( K \) model (Deardorff 1980), but now taking \( K \sim \Delta e^{1/2} \) and using an adjustment to allow smaller SFS length scales in stable stratification. The model included a conservation equation for the SFS turbulent kinetic energy \( e \), which Schumann (1975) had earlier used in simulations of turbulent duct flow. SFS models of this \( K-e \) type are now standard in LES codes for atmospheric applications. Moeng et al. (1996), for example, reported an intercomparison of 10 atmospheric LES codes, all of which used versions of this model.

The engineering fluid-mechanics community, which coined the name large-eddy simulation after Deardorff’s (1970) channel-flow study appeared, has had a rather different experience with LES. They applied it to a variety of flows and confirmed the soundness of its conceptual basis, but they also compared LES with direct numerical simulations of low Reynolds number turbulent flows (Clark et al. 1979). They found that the eddy-diffusivity SFS model represents the interaction between resolved and subfilter-scale turbulence well on average but poorly in detail. There ensued, and continues today, a long series of attempts to improve SFS modeling for engineering applications. A milestone here was the dynamic model (Germano et al. 1991), which attempts to compute the coefficient in the eddy-diffu-
sivity SFS model (9) dynamically as the calculation progresses. Meneveau and Katz (2000) discussed this and related approaches to SFS modeling for LES. Piomelli and Balaras (2002) reviewed recent progress in LES of boundary layer flows, focusing on the use of separate SFS models adjacent to the surface.

The mesoscale modeling community has evidently done less experimentation with their SFS models. It seems that virtually all mesoscale models use the $K$ closure, often with a conservation equation for the SFS turbulent kinetic energy.

d. Analysis of HATS observations

The Horizontal Array Turbulence Study (HATS; Sullivan et al. 2003) provided data useful for studying the behavior of the SFS flux conservation equations in the atmospheric surface layer. HATS employed the anemometer-array technique developed by Tong et al. (1998, 1999)—a pair of horizontal, crosswind arrays of sonic anemometers mounted parallel to the surface. Filtering in time (with Taylor’s hypothesis to convert to streamwise spatial filtering) and in the crosswind direction allows the turbulence fields to be decomposed into filtered and SFS parts. The data presented here were gathered in daytime conditions with slightly to moderately unstable conditions in runs ranging from 25 to 50 min long. Four array geometries were used in order to obtain a range of $l/\Delta$ values. We chose $l$ as the streamwise integral scale of the vertical velocity field, which the Kansas observations (Kaimal et al. 1972) showed is to a good approximation $5z$ ($z$ is the distance above the surface) under the conditions of our HATS runs; $\Delta$ is the scale of the filter in the horizontal plane.

We will briefly discuss some results for the SFS scalar-flux equation (18) with the scalar taken as potential temperature. In the LES limit each quantity in the flux-production term, which is expanded in Eq. (20), fluctuates about its ensemble-mean value. Figure 2 shows, for each component of scalar flux, the ratio of the rms (about the mean) value of its full, six-term production rate and the rms value of its gradient-diffusion part. For each of the SFS flux components this ratio is appreciably larger than 1.0, indicating that the fluctuating production term for SFS flux is not dominated by its gradient-diffusion part. Thus it appears that the simplest reasonable model of SFS scalar flux in the near-neutral surface layer is not the commonly used gradient-diffusion form (21), but rather the more general form (19).

The dashed line in Fig. 2 is the result of a simplified analytical calculation in the LES limit. The calculation approximates the $f_i$ in the production term by its gradient-diffusion form, assumes that the fourth moments that result when the expression is squared and averaged are related to second moments as for a Gaussian process, uses second-moment conservation equations to relate the third moments that result to second moments, and uses isotropic forms for second moments. As Fig. 2 shows, the numerical result of this calculation agrees well with the HATS data in the LES region, $l/\Delta \approx 10$.

We tested the more general SFS model (19) by comparing the SFS fluxes and scalar variance transfer rates it yields with those observed in HATS. In so doing we ignored the buoyancy term in the $f_3$ equation, whose net mean effect averaged about 20% of the mean value of the production term. In (19) we chose $T = Ce^{1/2}/\Delta$, with $C = 0.3$. We used the time series of $e$ and the gradients of filtered velocity and temperature observed in HATS to drive the model in its unsteady form, Eq. (26). In general, the advection term is also active in this equation, but it was not measured in the HATS experiment. Under horizontally homogeneous conditions it averages to zero, however, so its neglect here is presumably not serious. Figure 3 compares all three components of the run-averaged SFS temperature fluxes measured in HATS against the predictions of Eq. (26). The agreement is quite good.

Figure 4 shows a comparison of the run-averaged
values of the rate of temperature variance transfer, \(-2\bar{f_i}/\partial \bar{\alpha}_x\), from the model (26) and the HATS observations. Again the agreement is quite good. Figure 5 shows the fraction of the values of the rate of temperature variance transfer that are positive—that is, represent transfer from large scales to smaller—for the HATS observations and the model (26). Again the agreement is fairly good.

The ratio of the rms value of the six-term production rate of \(\bar{f_i}\) and the rms value of \(\partial \bar{f_i}/\partial t\) from HATS is plotted in Fig. 6. The rms time derivative is considerably larger than the rms production rate, particularly at the larger values of \(l/\Delta\). This indicates that the advection term in the full conservation equation (18) for \(f_i\) is the principal contributor to fluctuations in \(\bar{f_i}/\partial t\). Since the rms vertical advection is generally smaller than the rms production rate (Fig. 7), we conclude that horizontal advection is the primary source of these fluctuations. This suggests that without knowledge of the horizontal advection terms more detailed evaluations of SFS models, for example comparisons of measured and modeled time series, might not be possible.

e. Implications for numerical modeling

The SFS turbulence closures typically used in mesoscale models and LES today are of the same form—a scalar eddy-diffusivity model with \(K \sim e^{l/\lambda}$, with \(\lambda$ taken as \(l$ in mesoscale models and \(\Delta$ in LES. We showed from the HATS data, however, that the simplified conservation equation for SFS scalar flux implies a tensor eddy diffusivity, not a scalar one (Fig. 2).

In high-resolution LES, where \(l \gg \Delta\), the SFS model carries little turbulent flux; its principal role is extracting energy and scalar variance from the filtered scales. The scalar diffusivity SFS model is quite effective in this transfer role and it seems doubtful that the additional production terms included in the tensor-diffusivity model (19) would have any strong effects. This is consistent
with the early LES experience of Deardorff, who returned to the $K$-closure SFS model after several years of experience with SFS flux conservation equations, and the more recent experience of Schmidt and Schumann (1989), who commented that (except in inversion layers) their algebraic SFS model is of “minor importance” in high-resolution LES. Mason (1994) also mentioned the insensitivity of current LES to the SFS model, except near boundaries or in statically stable regions. Juneja and Brasseur (1999) discussed the deficiencies of the standard SFS model in reproducing near-surface structure. Thus, it seems that high-resolution LES in atmospheric applications would not benefit significantly from our more general SFS model except possibly very near surfaces and in stably stratified regions.

In coarse-resolution mesoscale modeling turbulent fluxes are carried entirely by the SFS model. Here the SFS models are typically developed, calibrated, and evaluated for $l \ll \Delta$, often in one-dimensional form (Ayotte et al. 1996). In effect they produce ensemble-mean fluxes, which in the atmospheric boundary layer are maintained by mean gradients in the vertical. The standard scalar eddy-diffusivity model can be tuned to represent these fluxes fairly well. Although the eddy diffusivity for conserved scalars in the convective boundary layer is not well behaved (Wyngaard and Weil 1991), a “nonlocal term” can be added (Stevens 2000) to accommodate much of this behavior as well. Thus, the tensor eddy-diffusivity model (19) is perhaps also not necessary in coarse-resolution mesoscale modeling.

But in LES near the surface, in most LES of severe storms (Bryan et al. 2003), and in very high resolution mesoscale modeling, $l$ is typically of the order of $\Delta$. In such applications, which lie outside the original design ranges of both mesoscale modeling and LES, the SFS model carries appreciable flux in an environment in which all three components of resolved gradients can be significant. In this “terra incognita” the tensor eddy-diffusivity SFS model could impact both LES and mesoscale modeling.

4. The terra incognita: Dynamical modeling with $l \sim \Delta$

a. A unified closure concept

Wyngaard (1982) and Bryan et al. (2003) have discussed qualitatively the behavior of the filtered equation of motion (4) as the filter scale $\Delta$ varies. To simplify our summary here we represent $\tau_\nu$ through a scalar eddy viscosity $K \sim e^{1/2}l^\prime$ and assume the filtered flow is statistically homogeneous in the horizontal and has velocity and length scales $U$ and $L$. The effective Reynolds number $Re$ of the filtered flow is therefore of order

$$Re = \frac{UL}{K} \sim \frac{UL}{e^{1/2}l^\prime}. \quad (33)$$

In the mesoscale limit $e^{1/2}$ and $l^\prime$ are $u$ and $l$, the scales of the turbulence, which in turn are of the order of (but less than) $U$ and $L$, the scales of the filtered flow. The Reynolds number of the filtered flow is then $O(1)$ and most likely below the value required for transition to turbulence. Thus, mesoscale model output fields are nonturbulent.

In the LES limit $l^\prime$ is the filter scale $\Delta$, which lies in the inertial subrange, so we can write

$$e = \int_{1/\Delta} E(\kappa) d\kappa \sim e^{1/2} \Delta^{1/3}. \quad (34)$$

With $e \sim u/\ell$ (Tennekes and Lumley 1972) this yields

$$e^{1/2} \sim u \left(\frac{l}{\Delta}\right)^{-1/3}, \quad K \sim e^{1/2} \Delta \sim u \Delta \left(\frac{l}{\Delta}\right)^{-1/3},$$

$$Re = \frac{UL}{K} \sim \frac{UL}{e^{1/2}l^\prime} \sim \frac{1}{\Delta} \left(\frac{l}{\Delta}\right)^{4/3}. \quad (35)$$

Since $l/\Delta \gg 1$, we expect LES output fields to be turbulent. The transition to turbulence evidently occurs in the scale region $l \sim \Delta$.

We have argued in section 3e that closures for SFS turbulence can plausibly have the same form in the mesoscale and LES limits. The only difference is the length scale of the SFS turbulence, $l$ in the mesoscale limit and $\Delta$ in the LES limit. As suggested by Cuxart et al. (2000), it is natural to use a single closure with its length scale transitioning between $l$ on the mesoscale side and $\Delta$ on the LES side (Fig. 8):

$$l^\prime = l, \quad \Delta \simeq l; \quad l^\prime = \Delta, \quad \Delta \simeq l. \quad (36)$$

b. The roles of buoyancy and turbulent transport

The experience with second-order closure (Zeman 1982) suggests that the conservation equations for SFS flux and energy described in section 3 need buoyancy
and turbulent-transport (third-moment flux divergence) terms to be optimally useful in geophysical applications. Including buoyancy is straightforward: through the Boussinesq approximation, for example, the equation of motion gains a buoyant acceleration term \( g\Theta/\Theta_0 \), with \( g \) the acceleration of gravity, \( \Theta_0 \) a background potential temperature profile, and \( \Theta \) a deviation from this profile. This generates buoyant-production terms in Eqs. (8) for SFS stress \( \tau_{ij} \) and (18) for SFS scalar flux \( f_i \). These are known to be quite important when \( l \ll \Delta \)—that is, in mesoscale and ensemble-mean modeling (Zeman 1982).

We can assess the importance of these buoyant-production terms when \( l \) is of the order of or greater than \( \Delta \) as follows. We define \( \theta(\Delta) \), the intensity scale of temperature fluctuations of spatial scale \( \Delta \), as the rms value of the fluctuating part of \( \Theta \) for filter scale \( \Delta \). Its counterpart for the velocity field is \( u(\Delta) \). Their Kolmogorov inertial-range scaling is (Tennekes and Lumley 1972)

\[
\begin{align*}
u(\Delta) & = f(\varepsilon, \Delta) = (\varepsilon \Delta)^{1/3}, \\
\theta(\Delta) & = g(\chi, \varepsilon, \Delta) = \chi^{1/2} e^{-16\Delta}/3.
\end{align*}
\]

These results hold also for \( \Delta \) in the energy-containing range, where the intensity scales are \( \theta \) and \( u \). That is, using \( \varepsilon \sim u^2/l \), \( \chi \sim \theta^2l \), Eq. (37) yields for \( l \)

\[
u(l) = u, \quad \theta(l) = \theta.
\]

It follows that

\[
\theta(\Delta) = \theta\left(\frac{l}{\Delta}\right)^{-1/3}, \quad u(\Delta) = u\left(\frac{l}{\Delta}\right)^{-1/3}.
\]

When the buoyant- and gradient-production terms in the SFS stress, energy, and scalar flux conservation equations are scaled with \( \Delta \), \( u(\Delta) \), and \( \theta(\Delta) \), their ratio becomes a scale-dependent turbulent Richardson number:

\[
\text{Ri}(\Delta) = \frac{g\theta(\Delta)}{\Theta_0[\mu(\Delta)]^2} = \frac{g\theta\left(l/\Delta\right)^{2/3}}{\Theta_0 u^2\left(l/\Delta\right)^{2/3}} = \text{Ri}_i\left(l/\Delta\right)^{-2/3}.
\]

Thus, if \( l \sim \Delta \), this turbulent Richardson number is of the order of \( \text{Ri}_i \), that for the energy-containing range, which in atmospheric turbulence can be \( O(1) \) in both stable and unstable stratification (Wyngaard 1992). If \( l \gg \Delta \), Eq. (40) says the direct effects of buoyancy on the SFS turbulence budgets are small.

Figure 9 shows the ratio of rms value of the buoyancy term in the \( f_i \) equation and the rms value of the sum of its six production terms, as evaluated from the HATS data. The relative importance of buoyancy effects decreases with increasing \( l/\Delta \), much as predicted.

The conservation equation for a filtered product of two turbulent variables \( (II, \text{say}) \) has the general form

\[
\frac{\partial II}{\partial t} + \frac{\partial II}{\partial x_i} = \frac{\partial III_i}{\partial x_i} + \cdots.
\]

The first term on the right, turbulent transport, can be

important, particularly in the mesoscale limit in unstably stratified conditions. There are two extremes in the modeling of such turbulent-transport terms in the ensemble-average framework (Zeman 1982). Reinterpreting these in the spatial-filtering context, the simplest model is gradient diffusion:

\[
III = -K \frac{\partial II}{\partial x_i} + K_i e^{l_i/2},
\]

with \( l_i \sim l \) and \( \Delta \) in the mesoscale and LES limits, respectively. The most complex approach is to write the rate equation for \( III \),

\[
\frac{\partial III}{\partial t} + \frac{\partial III}{\partial x_i} = \text{rhs},
\]

and calculate directly some of the terms on the right-hand side (including the buoyancy term), while modeling others. This approach can be quite effective in the unstable boundary layer (Zeman 1982). Again, the prescribed behavior of the length scale could allow a smooth transition of the turbulent transport model in the LES limit.

c. Caveat: An alternative averaging operator

We have assumed that the fields predicted by both mesoscale models and LES are defined through Leonard’s generalization (2) of Lilly’s spatial averaging operator (1). There is an alternative and quite different definition: that the fields are ensemble averages defined by

\[
\overline{F}(x, t) = \lim_{N \to \infty} \sum_{N=1}^{\beta} F(x, t; \beta).
\]

Here one averages over a large number of realizations of the same turbulent flow, holding position and time constant in the average. The ensemble average, also called the expected value, is the average of classical turbulence theory.
One could use the ensemble average in mesoscale modeling; indeed, at small enough \( l/D \) it can be indistinguishable from a spatial average. But the difference is profound at \( l/D \sim 1 \). In that \( l/D \) range spatial-averaged fields become turbulent, while ensemble-averaged fields are nonturbulent. Unless mesoscale modelers are inadvertently obtaining high-resolution but nonturbulent solutions through use of an incorrect turbulence closure (e.g., ensemble-averaged rather than spatially averaged), this is perhaps not an important issue in meteorology.

Ensemble-averaged models have traditionally been used to predict the dispersion of pollutants because a principal concern has been longer-term public health issues associated with releases of toxic effluents from continuous sources—for example, factory stacks. But to predict the dispersion of toxics from instantaneous releases (such as in terrorist attacks) one needs more than the ensemble-averaged result; one needs also the likely behavior in individual realizations (National Research Council 2003). The latter requires spatial-averaged models.

5. Summary and conclusions

Lilly’s (1967) conservation equation for SFS stress, and that derived later for SFS scalar flux, provide a foundation for SFS modeling for both mesoscale model and LES applications. These equations have several production terms, one of which produces the commonly assumed downgradient diffusion model of SFS flux. Our analyses of data from the HATS surface-layer array experiment indicate that the other SFS flux production terms can also be important. If so, this implies that the simplest SFS model consistent with the SFS flux conservation equations has a tensor rather than scalar eddy diffusivity. We suggest that the tensor nature of this diffusivity is probably not important in high-resolution LES or in low-resolution mesoscale modeling. It could be important in the terrain incognita, \( l \sim D \), which occurs in both very fine mesh mesoscale modeling and coarse-mesh LES.

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