1. INTRODUCTION

Experience with models and schemes for representing the effects of the unresolved motions in large-eddy simulations (LES) suggests that the near-wall and main flow domains require quite different treatments. Virtually all schemes make some special provisions for the near-wall representations. This is especially important when modeling field-scale flows, as the limited grid resolution throughout the domain places extra importance on the quality of the turbulence closure scheme.

A well-known problem in LES is the lack of agreement with logarithmic theory in the near-wall region. The goal of this work was to learn what logical steps and procedures are required for subfilter-scale (SFS) modeling to bring the simulated flow fields into agreement with theoretical expectations in the near-wall region. We examined a specific test case: the neutral, rotation-influenced, rough-wall, field-scale boundary-layer flow considered by Andren et al. (1994). A standard atmospheric mesoscale simulation code is used, namely, the Advanced Regional Prediction System (ARPS). Because this is a finite volume LES code for irregular terrain, spectral methods and sharp Fourier cutoffs in filters are not viable options. The only major modifications to the code are those associated with the new subfilter-scale models we have implemented.

The closure model implemented includes the series-expansion subfilter-scale turbulence model of Katopodes et al. (2000a,b). A priori tests for stratified homogeneous shear flow showed that the series model is superior to eddy viscosity models, as the series model has significantly improved correlations and ratios when compared to DNS values. However, when applied to this rough-wall boundary layer flow simulation, the series model requires augmentation. To better represent the near-wall region, we have adopted a hybrid approach. The series and Smagorinsky models are used in conjunction with the near-wall canopy stress term of Brown et al. (2001). Neutral boundary layer simulation tests show significantly improved results: the logarithmic velocity layer near the lower boundary is more closely reproduced, as compared to results with standard closure models.

In this paper, we present the framework for constructing a hybrid, or mixed, LES closure model. We then describe the implementation of this model and results from LES simulations of the neutral boundary layer, and close with a summary.

2. SFS AND SGS MOTIONS

ARPS employs spatially filtered compressible nonhydrostatic Navier-Stokes equations. For this paper, ARPS was operated in an incompressible mode (Xu et al. 1996).

Using Favre filtering to separate the density from the velocity, we define the SFS stress as

$$\tau_{ij} = \bar{\tau}_{ij} - \overline{u_i u_j}$$

where $\overline{u_i u_j}$ are the filtered velocity components. The filtered equations are not closed due to the nonlinear term $\overline{u_i u_j}$ included in $\tau_{ij}$.

To facilitate our understanding of this stress tensor and to improve turbulence models in the near wall region, it is useful to consider velocity partitioning schemes such as those of Carati et al. (2001), Zhou et al. (2001), and Hughes et al. (2001), and the spectral analysis of van Dijk and Duynkerke (2002). Figure 1 shows a schematic of a typical energy spectrum from a turbulent flow. The spectrum can be separated into three parts. The low wavenumber portion is well-resolved on the grid, and is contained in the velocity $\overline{u_i}$. The middle portion represents subfilter-scale motions that are between the filter and grid cutoffs. The last portion on the right contains subgrid-scale motions that cannot be resolved on the grid.

Following Carati et al. (2001), this velocity partitioning results in a decomposition for the LES stress tensor $\tau_{ij} = \tau_{A,ij} + \tau_{B,ij}$. The subgrid-scale (SGS) stress portion $\tau_{A,ij}$ depends on scales beyond the resolution domain of the LES, while the filtered-scale stress portion $\tau_{B,ij}$ depends on the differences between the exact and filtered velocity fields within the resolution domain, which we call subfilter-scale motions. This partitioning requires that the filter width be larger than the grid spacing. Note that in a continuous domain, $\tau_{A,ij}$ is zero, since there would be no contribution from subgrid-scale effects. The subfilter-scale component, $\tau_{B,ij}$ can theoretically be computed and does not need to be modeled; an infinite expansion in a series model for $\tau_{B,ij}$ would give the exact solution in this case. In a discrete domain, the contribution of $\tau_{ij}$, and thus $\tau_{A,ij}$, increases with decreasing grid resolution. Near the wall, the $\tau_{A,ij}$ terms become increasingly important.

3. CLOSURE MODELS

Using this framework for the turbulence closure, we can construct models for each component separately. For $\tau_{A,ij}$ we have examined, among others, multi-scale Smagorinsky models (Hughes et al. 2001) and the effect of the 4th-order numerical smoothing employed in ARPS to remove high-frequency noise and aliasing (which was not found to be significant). The small-scale Smagorinsky model was limited by discretization errors in the large-scale flow we are considering, and did not perform well.

Therefore, to model the unclosed term, $\tau_{A,ij}$, a simple gradient diffusion form is assumed:

$$\tau_{A,ij} = -2\nu_T S_{ij}$$

where $\nu_T$ is the eddy viscosity, and $S_{ij}$ is the resolved strain rate tensor. Despite the known shortcomings of this model, it is convenient to use when energy transfer to the...
subgrid scales is desired. A common treatment in LES is to use the Smagorinsky model (1963), which assumes

\[ \nu_T = (C_S \Delta)^2 (2\tilde{\Sigma}_{ij} \tilde{\Sigma}_{ij})^{1/2}, \]  

where \( C_S \) is the Smagorinsky coefficient, and \( \Delta \) is the grid spacing. Such gradient diffusion models are often applied to represent the entire stress tensor \( \tau_{ij} \), whereas here we apply the Smagorinsky model as part of a mixed model, so its contribution will not be as pronounced (see Zang et al. 1993).

For the stress term \( \tau_{ij} \), which can be expressed in terms of the resolved velocity, we have implemented the series model of Katopodes et al. (2000a), a task for which it is ideally suited. In the spirit of velocity estimation models (Geurts 1997, Domaradzki and Saiki 1997, Stolz and Adams 1999), the series model seeks to obtain an approximate expression for the unresolved variables and use these to calculate the SFS motions. This model uses successive inversion of a Taylor series expansion to express the unfiltered velocity in terms of the filtered (resolved) velocity. We then derive SFS models of arbitrary order of accuracy in the filter width, \( \Delta_f \), shown here to fourth order:

\[ \tau_{ij} = 2 \tilde{u}_i \tilde{u}_j - \tilde{u}_i \tilde{u}_j - \frac{\Delta_f^2}{24} \tilde{u}_i \nabla^2 \tilde{u}_j - \frac{\Delta_f^2}{24} \tilde{u}_j \nabla^2 \tilde{u}_i + \frac{\Delta_f^2}{24} \tilde{u}_i \nabla^2 \tilde{u}_i + \frac{\Delta_f^2}{24} \tilde{u}_j \nabla^2 \tilde{u}_j, \]  

where \( \Delta_f \) is the Smagorinsky coefficient, and \( \Delta_f \) is the grid spacing. Such gradient diffusion models are often applied to represent the entire stress tensor \( \tau_{ij} \), whereas here we apply the Smagorinsky model as part of a mixed model, so its contribution will not be as pronounced (see Zang et al. 1993).

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 et al. 1977). An anisotropic Gaussian filter is used, though an isotropic filter \( \Delta_f \) is shown here for simplicity (see Katopodes et al. 2000a) for further details. Other spatially compact filters give similar results, with a change in the expansion coefficients. It is important that the filter width be at least twice the size of the grid spacing, otherwise discretization errors will be as large as the effect of the SFS model (Ghosal 1996, Chow and Moin 2002). The series models also satisfy the full evolution equation for \( \tau_{ij} \) meaning that the effects of buoyancy, Coriolis forcing, pressure, and advection are naturally included in the model and do not need special treatment (Katopodes et al. 2000a).

This series model can be rewritten as

\[ \tau_{ij} = \frac{\Delta_f^2}{12} \frac{\partial \tilde{u}_i}{\partial x_m} \frac{\partial \tilde{u}_j}{\partial x_m}, \]  

which is equivalent to equation (4) to the fourth order in the filter width (Katopodes et al. 2000a). Equation 4 is similar to the model proposed by Clark et al. (1977). This modified Clark model is considerably simpler than equation (4) to implement numerically, so we adopt this as our model for \( \tau_{ij} \). This model has been used in a channel flow by Fischer and Iliescu (2001) to represent the entire turbulence term with good results. Winckelmans et al. (2001) performed a channel flow simulation using the modified Clark model together with the Smagorinsky model, as we do. However, both of these studies considered small-scale flow cases where viscous motions could be resolved near the wall, which is not possible in the atmospheric boundary layer. Vreman et al. (1996) also found that a mixed model with the original Clark model performed well for a small-scale temporal mixing layer.

Because of the resolution limitations present when simulating a field-scale flow, the turbulence model requires special treatment near the lower boundary which is rough. This mixed model using equations (2,3) and (5) has limitations near the solid lower boundary, where eddy sizes decrease much more rapidly than the grid spacing. Because the vertical grid-spacings are invariably smaller than the horizontal ones, \( 2 \times dx \) is the minimum vertical distance from the wall for eddies of the horizontal grid size to be resolved. This lack of resolution means that an additional stress term may be needed near the wall to represent these motions. Thus, in this near-wall region, such augmentation of the stress models is appropriate. Following Brown et al. (2001) and Cederwall and Street (2002), we implement a canopy stress model near the wall.

The canopy model can be expressed as a forcing term in the horizontal momentum equations as \(-C_c a(z) \tilde{u}_i \tilde{u}_j\), where \( i = 1, 2 \). Here \( C_c \) is a scaling factor and \( a(z) \) is a constant smoothing function which are both predetermined. Following Brown et al. (2001), we choose \( a = \cos^2(\pi z/h_c) \) for \( z < h_c \), where \( h_c \) is the canopy height. Above the canopy, we set \( a = 0 \). This function \( a(z) \) allows for a smooth decay of the forcing canopy function as the specified canopy height is approached.

In the code, the canopy force is treated as part of the turbulence closure stress term, and therefore is integrated numerically using the trapezoidal rule from

\[ \tau_{i,can} = - \int C_c a(z) \tilde{u}_i \tilde{u}_j dz, \]  

where the integration constants are chosen so that \( \tau_{i,can} = 0 \) at the top of the canopy. This stress is then directly added to the \( \tau_{ij} \) terms contributed by the other model components. Brown et al. (2001) choose a constant value for \( C_c \) so that the velocity at the top of the canopy matches that from experimental measurements. Cederwall (2001) selected \( C_c \) such that the canopy model augmented the total stress at the first grid point above the wall to make it equal to the local bottom shear stress. Instead we allow \( C_c \) to be locally proportional to the bottom shear stress in each horizontal direction. The proportionality factor is chosen to allow the canopy to provide the necessary augmentation that will yield logarithmic mean velocity profiles near the wall.

4. NEUTRAL BOUNDARY LAYER SIMULATIONS

To test the performance of the closure models, we use the ARPS code to simulate a neutral boundary layer flow.
case similar to that of Andren et al. (1994). ARPS was developed and tested at the Center for Analysis and Prediction of Storms at the University of Oklahoma over the last decade. Details on the ARPS code can be found in Xue et al. (2001). The equations have been slightly modified to make them closer to the incompressible case studied by Andren et al. (1994), as detailed in Xu et al. (1996).

The no-slip condition cannot be applied at the bottom boundary in atmospheric boundary layer simulations because the surface is rough. Hence, the top and bottom boundaries are treated as rigid or free-slip boundaries, and surface fluxes are parameterized to account for the influence of the rough bottom surface. The ARPS code parameterizes the momentum fluxes at the surface using a logarithmic drag law (with stability-dependent similarity options).

The flow is driven by a constant geostrophic pressure gradient which would balance a geostrophic wind of \((U_g, V_g) = (10, 0) \text{ m/s}\). The Coriolis parameter, \(f\), is set equal to \(9 \times 10^{-5}\). The bottom roughness is set to 0.1\(m\). At the lateral boundaries, periodic conditions are used for this idealized flat-terrain study. This configuration results in an Ekman-like spiral for the mean velocities. The grid size is \(40 \times 40 \times 40\) with grid spacings of \(32m \times 32m\) in the horizontal. In the vertical, a stretched grid is used, with \(8m\) spacing near the bottom and up to \(104m\) near the top of the domain, giving an average spacing of \(37.5m\). The anisotropic filter for the modified Clark model was applied at twice the grid spacing, in computational space. Simulations were run for 100000\(s\) (approximately 10 inertial time periods, \(tf\)) with a 0.5\(\text{s}\) large timestep, and 0.05\(\text{s}\) small timestep.

The mean velocity profile is expected to be logarithmic in the lowest region of the boundary layer, as can be shown from similarity theory (Blackadar and Tennekes 1968). As noted by Andren et al. (1994), one of the many short-comings of the widely-used eddy viscosity models is their failure to produce logarithmic profiles. Such errors near the wall can affect the entire flow solution. A convenient measure of the model’s performance in this respect is the non-dimensional velocity gradient, \(\Phi\), which is defined as

\[
\Phi = \frac{\kappa z}{u_*} \sqrt{\left( \frac{\partial <u>}{\partial z} \right)^2 + \left( \frac{\partial <v>}{\partial z} \right)^2}. \tag{7}
\]

Here \(\kappa\) is the von Kármán constant, chosen to be 0.4; \(u_*\) is the surface friction velocity defined by \(u_* = \sqrt{\frac{\overline{uv}_0}{\overline{v}_0}}\) \(^{1/4}\), where \(\overline{uv}_0\) and \(\overline{v}_0\) are the total stresses at the lower boundary. For the parameters chosen, \(u_*\) is found to be approximately 0.4. In a logarithmic region, \(\Phi = 1\), which we expect for approximately the first 200\(m\) above the wall. Vertical profiles are averaged horizontally in space (denoted by the brackets \(<\>\)), as well as in time over the last 20000\(s\) of the simulation, using data taken at 1000\(s\) intervals.

Stress profiles for \(uw\) are shown in Figure 2 where the contribution of each component in the closure model can be seen. The total stress is approximately linear, as expected in a boundary layer flow. The stress profiles are also shown on a log plot to magnify the region near the wall. The influence of the canopy model decreases as the canopy top is approached, which is selected to be \(4 \times dz\) (128\(m\)), or equivalent to the minimum well-resolved horizontal eddy size beneath the filter. We obtain good results when we choose the canopy coefficient \(C_c\) so that the canopy model contributes an amount equal to half the wall stress at the first grid point above the wall. We also apply damping to the canopy model using \((1 - \exp(-z/d))^2\) (with \(d = 15m\)) very near the wall to slightly reduce the canopy effect there as it was found to be too large. The Smagorinsky coefficient is chosen as \(C_S = 0.21\), the standard value used in the ARPS code. The modified Clark term decays to zero naturally at the wall in the presence of the other two model components.

Profiles of \(\Phi\) are shown in Figure 3. We compare our results with the hybrid closure model to those using the standard Smagorinsky eddy viscosity model. We see that the overshoot in the value of \(\Phi\) reaches 1.8 for the traditional Smagorinsky model, indicating the model provides excessive shear near the surface. When the modified Clark, canopy, and Smagorinsky models are used together, the overshoot in the value of \(\Phi\) near the wall from the Smagorinsky model is compensated by the designed tendency for the canopy model to produce \(\Phi\) values less than unity. In addition, the modified Clark component is of scale-similar form, and thus allows backscatter, or energy 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 atmospheric boundary layer (Mason and Thomson 1992), and aids in achieving a logarithmic mean velocity profile. Except for at the lowest point, values of \(\Phi\) within 0.2 of the ideal are obtained using the hybrid model, which represents a significant improvement. With a subset of only one or two components of this hybrid model (e.g., Smagorinsky and series models without the canopy), the results are not as good.

5. CONCLUSIONS

Our conclusion is that the context provided by Carati et al. (2001), is useful and leads to insights about model behavior. We are able to achieve improved non-dimensional shear \(\Phi\) profiles by a systematic use of the models cited above. We have found that when applied to simulations of the atmospheric boundary layer, the SFS series model (Katopodes et al. 2000a,b) needs augmentation because of finite grid resolution, and further special treatment at the lower rough boundary. The Smagorinsky model has been used to provide necessary dissipation, without incurring the expected drawbacks of this model as it is used in conjunction with a scale-similarity model. Near the earth’s surface, resolution is generally not adequate to resolve many of the turbulent motions and a supplemental model such as the canopy model improves the results. Further work is required for a careful assessment of the canopy model, as a more robust selection process for the coefficients in this model is desired.

6. ACKNOWLEDGMENTS

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7. REFERENCES


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