A modulated gradient model for large-eddy simulation: Application to a neutral atmospheric boundary layer

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The subgrid-scale (SGS) parametrization represents a critical component of a successful large-eddy simulation (LES). It is known that in LES of high-Reynolds-number atmospheric boundary layer turbulence, standard eddy-viscosity models poorly predict mean shear in the near-wall region and yield erroneous velocity profiles. In this paper, a modulated gradient model is proposed. This approach is based on the Taylor expansion of the SGS stress and uses local equilibrium hypothesis to evaluate the SGS kinetic energy. To ensure numerical stability, a clipping procedure is used to avoid local kinetic energy transfer from unresolved to resolved scales. Two approaches are considered to specify the model coefficient: a constant value of 1 and a simple correction to account for the effects of the clipping procedure on the SGS energy production rate. The model is assessed through a systematic comparison with well-established empirical formulations and theoretical predictions of a variety of flow statistics in a neutral atmospheric boundary layer. Overall, the statistics of the simulated velocity field obtained with the new model show good agreement with reference results and a significant improvement compared to simulations with standard eddy-viscosity models. For instance, the new model is capable of reproducing the expected log-law mean velocity profile and power-law energy spectra. Simulations also yield streaky structures and near-Gaussian probability density functions of velocity in the near-wall region. It is found that using a constant coefficient of 1 yields a slightly excessive SGS dissipation, which is corrected when the coefficient is modified using the above mentioned correction. \(\copyright\) 2010 American Institute of Physics.

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I. INTRODUCTION

Large-eddy simulation (LES) of anisotropic turbulent flows has been an active and challenging field since the 1960s. In LES, large scales are explicitly resolved, while effects of subgrid scales (SGSs) are parametrized. SGS modeling is necessarily based on simple assumptions and phenomenological theories. Even though most SGS models assume a universal behavior of small scales, this assumption often breaks down due to flow anisotropy affecting the unresolved scales, for instance near the surface in high-Reynolds-number boundary layer flows. As a result, several studies\(^1\)–\(^4\) have shown that simulation results are highly sensitive to the SGS model as well as to the grid resolution.

Most simulations of atmospheric boundary layer (ABL) turbulence have been achieved using eddy-viscosity-based SGS models.\(^5\)–\(^7\),\(^11\) The eddy-viscosity closure assumes a one-to-one correlation between the SGS stress tensor and the strain rate tensor, and locally employs the same eddy viscosity for all directions. However, \textit{a priori} analysis of velocity fields obtained from experiments\(^8\)–\(^9\) and direct numerical simulations (DNSs)\(^10\),\(^11\) confirmed the low correlation between the SGS stress tensor and the strain rate tensor. Studies of Khanna and Brasseur,\(^12\) Juneja and Brasseur,\(^13\) and Porté-Agel \textit{et al.}\(^3\) have also shown that on coarse grids eddy-viscosity models may induce large errors because they are not able to account for the strong flow anisotropy in the near-wall region. Moreover, eddy-viscosity models do not have the same rotation transformation properties as the actual SGS stress tensor, which is not material frame indifferent (MFI). Recent studies\(^14\),\(^15\),\(^11\),\(^16\) revisited the importance of the MFI-consistency of the modeled SGS stresses. In LES of mesoscale and large-scale atmospheric turbulence including planetary rotation, eddy-viscosity models induce extra errors and yield unsatisfactory results, such as the incapability of capturing cyclone/anticyclone asymmetry in favor of cyclone.\(^16\) In addition, eddy-viscosity models are by construction fully dissipative, and do not allow energy transfer from unresolved to resolved scales. However, such inverse energy transfer is known to occur, especially in anisotropic turbulence.\(^17\),\(^18\)

Gradient models, also referred to as nonlinear models, have been proposed since the late 1970s.\(^19\) They are based on the Taylor expansion of the SGS stresses: \(\tau_{ij} = \bar{u}_i \bar{u}_j - \bar{u} \bar{u}_i + O(\Delta^4)\), where the gradient term is \(\tilde{G}_{ij} = (\Delta^2/12) \times [(\partial \bar{u}_i / \partial x_k)(\partial \bar{u}_j / \partial x_k)]\) for isotropic Gaussian filter of size \(\Delta\). The gradient approach has several important advantages:\(^8\),\(^20\),\(^11\) (i) it does not require an extra filtering, (ii) it satisfies Galilean invariance and the modeled stress

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tensor is MFI-consistent with the actual SGS stress tensor, (iii) at the \textit{a priori} test level, the analysis has shown the modeled SGS stresses exhibit good correlations with the actual SGS stresses over a wide range of filter sizes, (iv) it only relies on local velocity gradients and thus is easy to be applied to turbulent flows in complex geometries, and (v) it allows energy transfer from small to large scales. However, the standard gradient model has also one important limitation: when implemented in LESs, it hardly dissipates small-scale turbulence, as a result, simulations become numerically unstable.

Different schemes have been introduced to resolve this insufficient small-scale dissipation issue for high-correlation models. In 1980, Bardina \textit{et al.} \cite{Bardina1980} introduced a mixed procedure, which is a linear combination of a scale-similarity model and an eddy-viscosity model. Vreman \textit{et al.} \cite{Vreman1996} and Lu \textit{et al.} \cite{Lu2010} also applied a similar mixed procedure with the gradient model and showed that mixed gradient models are able to capture disequilibrium and anisotropy effects. In 1994, Liu, Meneveau, and Katz \cite{Liu1994} revisited this energy cascade issue and recommended another meaningful choice, a clipping procedure, to control the amplitude of backward cascade induced by the model. Inconveniently, Vreman \textit{et al.} \cite{Vreman1996} reported that the modified (coupled with clipping) gradient model still does not provide sufficient SGS dissipation in simulations of mixing flows. We also found a similar limitation of this scheme in simulations of ABL turbulence.

In an effort to improve the correlation as well as the magnitude of the SGS stress, Pomraning and Rutland\cite{Pomraning1981} introduced a one-equation scheme, which models the SGS stresses as 

\[
\tau_{ij} = k_{sge}C_{ij}.
\]

The SGS kinetic energy, \(k_{sge} = (1/2) \times \left( u_i \partial_i u_j - \bar{u}_i \bar{u}_j \right) \), is calculated by solving an additional prognostic equation. The resulting model is consistent with the fact that dissipation rate is non-negative. The SGS kinetic energy is evaluated using the resolved velocities. To do that, we use the “local” equilibrium hypothesis, which assumes a balance between SGS energy production \(P\) and dissipation rate \(\varepsilon\). SGS energy production is defined as

\[
P = -\tau_{ij} \partial_i \bar{u}_j = -\varepsilon \bar{S}_{ij}.
\]

A simple evaluation of kinetic energy dissipation is \(\varepsilon = C_e (\bar{k}_{sge} / \Delta)\), and the coefficient is assumed to be \(C_e = 1\) based on previous studies.\cite{Vreman1996, Lu2010} Using the proposed model formulation [Eq. (1)] together with the local equilibrium hypothesis, one may obtain

\[
k_{sge} = (4\Delta^2/C_e^2)\left[ -\bar{G}_{ij} \bar{G}_{kk} \bar{S}_{ij} \right]^2 + \varepsilon = (8\Delta^2/C_e^2) \times \left[ -\bar{G}_{ij} \bar{G}_{kk} \bar{S}_{ij} \right].
\]

To ensure numerical stability, no local energy transfer from unresolved to resolved scales is allowed, which is consistent with the fact that dissipation rate is non-negative, and thus

\[
k_{sge} = \begin{cases} 
\frac{4\Delta^2}{C_e} \left( -\frac{\bar{G}_{ij} \bar{S}_{ij}}{\bar{G}_{kk}} \right)^2 & \text{if } \bar{G}_{ij} \bar{S}_{ij} < 0, \\
0 & \text{otherwise.}
\end{cases}
\]

It is important to point out that the value of \(C_e = 1\) is based on the assumption of an averaged energy balance between SGS energy production and dissipation rate in the inertial subrange of high-Reynolds-number turbulence (see Chap. 13 of Ref. 28). Considering that the clipping procedure eliminates the contribution of inverse energy transfer \((P < 0)\), a value of \(C_e = 1\) is likely to overestimate the SGS energy transfer rate. Therefore, it is of interest to have a correction coefficient \(C\) to modify \(C_e\) such that \((\varepsilon_c)\) can represent the actual dissipation rate more accurately, where the subscript “\(c\)” denotes conditional average requiring \(-\bar{G}_{ij} \bar{S}_{ij} \geq 0\). In the case of homogeneous boundary layers, like the one considered here, averaging is performed over homoge-
neous directions (horizontal planes). A simple solution for $C$ is obtained, based on information contained in the resolved scales,

$$C = \sqrt{\left(\frac{-\overline{G_{ij}} \overline{S_{ij}}}{G_{kk}}\right)^3} \cdot \left(\frac{-\overline{G_{ij}} \overline{S_{ij}}}{G_{kk}}\right)^{-1}. \tag{4}$$

Thus, an adjusted SGS kinetic energy to be used in the modulated gradient model is

$$k_{srg} = \begin{cases} \frac{4\Delta^2}{(C_s C)^2} - \frac{\overline{G_{ij}} \overline{S_{ij}}}{G_{kk}}^2 & \text{if } \overline{G_{ij}} \overline{S_{ij}} < 0, \\ 0 & \text{otherwise.} \end{cases} \tag{5}$$

In summary, Eqs. (1) and (3)–(5) form the basis of the new modulated gradient model. It should be noted that the model retains advantageous features of the standard gradient model and, in addition, it is expected to have improved dissipation characteristics. Next, the model is tested in simulations of the well-established case of a high-Reynolds-number turbulent boundary layer flow over a homogeneous surface. To isolate the effect of the correction given by Eq. (4) on the model performance, two versions of the model are tested: (i) a “baseline” model that uses Eq. (3) [same as Eq. (5) with $C=1$] to estimate the SGS kinetic energy and (ii) a “corrected” model that uses Eq. (4) to compute the correction coefficient $C$ and uses Eq. (5) to estimate the SGS kinetic energy.

### III. PROBLEM FORMULATION

We use a modified LES code which has been used for other studies.\textsuperscript{29,30,31,33} The code solves the filtered Navier–Stokes equations,

$$\frac{\partial \overline{u_i}}{\partial t} + \frac{\partial \overline{u_j} \overline{u_i}}{\partial x_j} = - \frac{\partial \overline{p}}{\partial x_i} + \frac{\partial \overline{f_i}}{\partial x_j}, \tag{6}$$

where $\overline{p}$ is the effective pressure, $\overline{f_i}$ is a forcing term, and the SGS stress tensor is $\overline{\tau_{ij}}=\overline{u_i} \overline{u_j} - \overline{u_i} \overline{u_j}$. The simulated flow is driven by a constant pressure gradient $-u_0^2/H$ in the streamwise direction. Since the Reynolds number is high, no near-ground viscous processes are resolved, and the viscous term is neglected in the momentum equation. The paper focuses on the case of neutral stability conditions, thus no additional terms concerning buoyancy effects and rotational effects are considered.

The numerical setup is classical and has been used for many applications and model assessments (e.g., Refs. 30 and 3). The simulated ABL is horizontally homogeneous. The horizontal directions are discretized pseudospectrally and vertical derivatives are approximated with second-order central differences. The grid planes are staggered in the vertical with the first vertical velocity plane at a distance $\Delta z = H/(N_z - 1)$ from the surface, and the first horizontal velocity plane $\Delta z/2$ from the surface. The height of the computational domain is $H=1000$ m, and the horizontal dimensions of the simulated volume are $L_x=L_y=2uH$. The domain is divided into $N_x$, $N_y$, and $N_z$ uniformly spaced grid points. We carried out simulations with resolutions of $N_x \times N_y \times N_z=24 \times 24 \times 24$, $32 \times 32 \times 32$, $48 \times 48 \times 48$, $64 \times 64 \times 64$, $96 \times 96 \times 96$, and $128 \times 128 \times 128$. The filter width is computed using the common formulation $\Delta = (\Delta x \Delta y \Delta z)^{1/3}$, where $\Delta x = L_x/N_x$ and $\Delta y = L_y/N_y$. The corresponding aliasing errors are corrected in the nonlinear terms according to the $3/2$ rule.\textsuperscript{34} The time advancement is carried out using a second-order-accurate Adams–Bashforth scheme.\textsuperscript{34} All simulations reached their statistically steady state.

The upper boundary conditions are $\partial \overline{u_i}/\partial z = 0$, $\partial \overline{u_j}/\partial z = 0$, and $\overline{u_i} = 0$. At the bottom surface, the instantaneous wall stress is related to the velocity at the first vertical node through the application of the Monin–Obukhov similarity theory.\textsuperscript{35} Although this theory was developed for mean quantities, it is common practice\textsuperscript{6} in LES of atmospheric flows to use it for instantaneous fields as follows:

$$\tau_{i|w} = -u_*^2 \frac{\overline{u_i}}{U(z)} = -\left(\frac{U(z)\kappa}{\ln(z/z_0) - \Psi_M}\right)^2 \frac{\overline{u_i}}{U(z)} \quad (i = 1, 2), \tag{7}$$

where $\tau_{i|w}$ is the instantaneous local wall stress, $u_*$ is the friction velocity, $z_0$ is the roughness length, $\kappa$ is the von Kármán constant, $\Psi_M$ is the stability correction for momentum, and $U(z)$ is the plane averaged resolved horizontal velocity. We adopt $\kappa=0.4$ in this paper. In the literature, there are some variations on this value but generally they are within 5%. We take $u_* = 0.45\text{ m s}^{-1}$ and $z_0 = 0.1\text{ m}$, which is a similar setup as some previous studies.\textsuperscript{1,29,3} In the case of neutral stability, $\Psi_M=0$. The instantaneous resolved horizontal velocity is computed at a height of $z=\Delta z/2$. We use this classical scheme in order not to confuse effects with the SGS modeling which is the focus of the present work. Further, to reduce the error incurred by using a finite-difference approach to compute the vertical derivative of the nonlinear convective term $\overline{u_j} \overline{\tau_{ij}}/\partial z$, we employed a correction factor\textsuperscript{3} at the bottom layer. This correction only improves the mean velocity profile in the lower levels, and appears to have no effect on other statistics.

### IV. RESULTS AND DISCUSSION

A series of large-eddy simulations with varying grid resolutions has been carried out using the baseline model, as well as the corrected model. For simplicity, “simulation using the baseline model” is abbreviated to “baseline simulation,” and “simulation using the correct model” is abbreviated to “corrected simulation.” Mean and turbulent statistics are gathered after statistically steady states were reached. In some subsections, we take the $64 \times 64 \times 64$-node simulation and the $128 \times 128 \times 128$-nodes simulation as base cases to present results. Also, we adopt the most commonly used symbols ($u$, $v$, and $w$) for the three velocity components.

#### A. Comparison with similarity theory predictions

In fluid dynamics, the log-law, which was first published by von Kármán,\textsuperscript{36} states that the mean streamwise velocity at a certain point in a turbulent boundary layer is proportional to the logarithm of the distance from that point to the wall. It
is a self-similar solution for the mean velocity parallel to the wall. The theory has been experimentally confirmed in a number of field experiments such as the Kansas experiment and represents one of the most firmly established results against which new SGS models should be compared. For high-Reynolds-number boundary layer flows, where viscous effects can be negligible, it can be written as

$$\frac{\langle u \rangle}{H} = \frac{u}{H} \ln \frac{z}{z_0},$$

where $\langle \cdot \rangle$ represents time and horizontal averaging in our study. The aerodynamic roughness, $z_0$, is necessarily nonzero since the log-law does not apply to the viscous sublayer.

Though the log-law is a good approximation for the velocity profile of boundary layer turbulence, it is only technically applicable to the so-called surface layer, which occupies the lowest 10%–20% of the flow in the ABL. The mean streamwise velocity profile from different resolution baseline simulations and corrected simulations are presented in Figs. 1 and 2. Clearly, the mean streamwise velocity results are close to the expected log-law profile (straight dashed line). In the near-wall region, corrected simulations yield $\langle \tilde{u} \rangle$ closer to the log-law, compared to baseline simulations. Table I presents relative errors of $\langle \tilde{u} \rangle$ at a height of $z/H=0.1$. All simulations yield small discrepancies with the log-law (relative errors within 5%). Baseline simulations have a tendency of increasing accuracy with increasing resolution. For the 96$^3$ case and the 128$^3$ case, corrected simulations yield slightly larger error magnitudes. This may be caused by the combined effects of the bottom boundary condition and the SGS modeling. However, corrected simulations consistently show smaller discrepancies and weaker resolution dependence.

To more rigorously evaluate model performance, one may examine the values of the mean nondimensional vertical gradient of the streamwise velocity $\Phi=(\kappa z/u_*)(d\langle \tilde{u} \rangle/dz)$ as a function of vertical position. Theoretically, this nondimensional vertical gradient is unity in the surface layer. In 1994, Andren et al. performed an extensive comparison of various LES codes using the standard Smagorinsky model with wall damping and other eddy-viscosity models. In the surface layer, from $z/H=0$ to $z/H=0.2$, their values of $\Phi$ were mostly larger than 1.2, and some simulations yielded $\Phi=2$. Similar overshoots in $\Phi$ reaching over 1.5 for the standard Smagorinsky model have been observed in many studies. It appears that the standard Smagorinsky model is too dissipative, removing too much kinetic energy from the resolved field and generating a near-linear profile in the surface layer, which bears a large value of $\Phi$. The values of $\Phi$ resulting from the present simulations are presented in Figs. 3 and 4. The modulated gradient model yields a value of $\Phi$ that remains close to 1 in the surface layer, indicative of the expected logarithmic velocity profile. It should be noted that using the baseline model, the nondimensional vertical gradient is slightly underestimated for the lowest two to three grid points (with the lowest value of about 0.85), which leads

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**FIG. 1.** Normalized mean streamwise velocity profile in a semilogarithmic scale: (a) results from low-resolution baseline simulations and (b) results from high-resolution baseline simulations. The dashed line corresponds to the classical log-law with $\kappa=0.4$.

**FIG. 2.** Normalized mean streamwise velocity profile in a semilogarithmic scale: (a) results from low-resolution corrected simulations and (b) results from high-resolution corrected simulations. The dashed line corresponds to the classical log-law with $\kappa=0.4$. 
to the slight underestimation of the average velocity as shown in Fig. 1 and Table I. The corrected model appears to remove this bias.

Next, Fig. 5 shows the vertical distribution of the averaged value of the correction coefficient computed using Eq. (4) for different resolution simulations. The value of $C$ is larger than 1 due to the fact that the denominator in Eq. (4) is always smaller than the numerator, since all negative values of the SGS energy transfer rate have been clipped to zero. This correction compensates for the overestimation of the SGS energy transfer rate associated with the use of the clipping procedure. $C$ has values that increase with height and range from about 1.2 near the surface to 1.6 away from the surface. Note that the collapse of all curves indicates that the value of $C$ is dependent on $z/\Delta$ only.

B. Energy spectra

It is important to test the ability of LES to accurately reproduce the main spectral characteristics of the resolved field. Spectra of velocity fields in turbulent boundary layers are known to exhibit three distinct spectral scaling regions: the energy-production range, the inertial subrange, and the dissipation range. In the case of LES of high-Reynolds-number boundary layers, the dissipation range is not resolved and, therefore, it will not be considered here. It is well known that the energy spectra of three wind components satisfy the Kolmogorov $-5/3$ power-law in the inertial subrange, i.e., the range of relatively small, isotropic scales that satisfy $k_1z \gtrsim 1$, where $k_1$ is the streamwise wavenumber. Also, laboratory and field measurements of boundary-layer turbulence show that in the energy-production range,
corresponding to scales larger than the distance to the surface \( (k_{1}z \leq 1) \) and smaller than the integral scale, spectra of the streamwise velocity often follow a \(-1\) power law, i.e., they are proportional to \( k_{1}^{-1} \).

Previous LES studies examined model performance regarding energy spectra, and limitations have been found for traditional SGS models. The spectra of the streamwise velocity obtained using the standard Smagorinsky model decay significantly faster (some simulations yield spectrum slopes as large as \(-7\)) than the expected \(-1\) power law in the near-wall region.\(^{1,40,3}\) Within the constraints of the Smagorinsky model, this type of spectrum means that the model dissipates kinetic energy at an excessive rate. The resulting spectra obtained using the dynamic Smagorinsky model, on the other hand, decay too slowly (the spectrum slope is close to \(-0.5\)) in the near-wall region.\(^{3}\) This is likely to be due to the fact that the dynamic procedure samples scales near and beyond the local integral scale, at which the assumption of scale invariance of the coefficient (on which the model relies) breaks down, leading to an underestimation of the Smagorinsky coefficient near the surface.\(^{3}\) The lower coefficient then yields lower energy dissipation rate and pile-up of energy at high wavenumbers. It is also found that, in the inertial subrange, the dynamic Smagorinsky model may yield a streamwise velocity spectrum slope shallower (close to \(-0.8\)) than \(-5/3.\(^{7}\)

Figures 6 and 7 show the normalized spectra of the simulated streamwise and vertical velocity, computed at different heights. Results are presented for the two model versions (with the baseline simulation results on the top panels, and with the corrected simulation results on the bottom panels) as well as two different resolutions (the \(64^3\) resolution results on the left panels and the \(128^3\) resolution results on the right panels). Spectra are calculated from one-

![Graph](image-url)
dimensional Fourier transforms of the velocity component and then are averaged both horizontally and in time. Streamwise wavenumber is normalized by the height and spectrum magnitude is normalized by \( u/H \). It should be noted that the spectra of the spanwise velocity are similar to the spectra of the streamwise velocity. The baseline model leads to spectra that are consistently too steep at large wave numbers. This is consistent with the feature that the baseline model overestimates the dissipation rate. This excessive dissipation is more evident in the coarser resolution baseline simulation. Results are clearly improved for both resolutions when the correction given by Eq. is used. In that case, in the inertial subrange all the normalized spectra show a better collapse and are in good agreement with the \( 5/3 \) power law. The improvement in the dissipation characteristics of the model due to the correction can be explained considering that the relatively larger values of \( C \) (see Fig. 5) provided by the correction lead to relatively smaller values of \( \tau_{ij} \), and, consequently, SGS energy transfer rates. For scales larger than the distance to the surface \( (k_1z \approx 1) \), the slope of the spectra of the streamwise velocity is slightly lower than \(-1 \) (close to \(-0.7 \)). The spectra of the vertical velocity differ from the spectra of the streamwise velocity. As shown in Fig. 7, there is no clear \(-1 \) power-law region; instead the spectra are flat in the near-wall region. This finding is consistent with the expected distribution supported by theoretical and experimental studies.

C. Flow visualization

A few remarks must be made regarding the ability of LES calculations to capture the structure of turbulence. We define three components of the resolved velocity fluctuation as \( \vec{u}' = \vec{u} - \langle \vec{u} \rangle \). Coherent streamwise elongated "streaks" of \( \vec{u}' \) are ubiquitous in turbulent boundary flows and have been repeatedly observed in a variety of contexts. Figures 8(a), 8(c), and 8(e) present instantaneous contours of \( \vec{u}'/u_\tau \) on a horizontal plane obtained from the 64\(^3\) baseline simulation, the 128\(^3\) baseline simulation, and the 128\(^3\) corrected simulation, respectively. Elongated structures of high-speed and low-speed \( \vec{u}' \) are evident. The contours of \( \vec{u}'/u_\tau \) are more diffused in the 64\(^3\) baseline simulation. As expected, the 128\(^3\) baseline simulation shows finer structures. This observation is consistent with other LES studies of turbulent boundary flows. Low-speed streaklike structure is closely related to vortical motions and corresponds to streamwise momentum being transported away from the wall. Figures 8(c) and 8(e) show that the low-speed regions appear more concentrated and elongated (often spanning the entire streamwise domain in our simulations) than the high-speed regions. This finding is consistent with LES and DNS results and recent experimental measurements. Moreover, Figs. 8(c) and 8(e) reveal a clear difference between the structure of the streaks simulated with both models under consideration. Using the correction coefficient yields
simulated streamwise velocity fields that have more small-scale structure. This is consistent with the fact that the baseline model dissipates too much energy (as pointed in the energy spectra subsection), thus overly smoothing the velocity fields at the smallest resolved scales.

Figures 8(a), 8(c), and 8(e) present instantaneous contours of $\bar{u}'/u_*$ on a vertical plane obtained from the 64$^3$ baseline simulation, the 128$^3$ baseline simulation, and the 128$^3$ corrected simulation, respectively. The strong vertical coherence of the updrafts and downdrafts is evident. Small plumes originate near the ground, and some of them are suppressed by strong downdrafts, while others merge with their neighbors to form larger stronger updrafts. The updraft regions are stronger and more spatially coherent than the downdraft regions, and also the near-wall low-speed streaks as shown in Figs. 8(a), 8(c), and 8(e) are kinematically tied to the presence of strong updrafts. These turbulent structures are consistent with results in other studies.49,12 Like in the case of the horizontal velocity fields, using the correction coefficient yields simulated vertical velocity fields that have more small-scale structure.

D. PDF of velocity fluctuations

Based on the central limit theorem, probability density functions (PDFs) for turbulent velocities are near-Gaussian. Experimental studies51,52 confirmed this statement in turbulent boundary layer flows, particularly near the wall. Figure 9 examines the PDF of $\bar{u}'/u_*$, $\bar{v}'/u_*$, and $\bar{w}'/u_*$ at a height of $z/H=0.1$ obtained from simulations using the two model.
versions at two resolutions. To accentuate the PDF tails, a log ordinate axis is used. PDF plots are very weakly skewed and the approach to Gaussian distribution is evident. To quantitatively examine their statistical characteristics, the skewness and flatness factors are shown in Figs. 10 and 11. The magnitude of skewness factors is generally smaller than 0.5, indicating a weakly skewed probability distribution. As required by the spanwise symmetry of the flow, the skewness of $\tilde{u}'$ must be nearly zero, and current simulations demonstrate this symmetry reasonably well as seen in Fig. 10(b). The skewness of $\tilde{u}'$, as revealed through previous experiments and LES studies, is mostly negative indicating a predominance of negative streamwise velocity fluctuations accompanying more elongated low-speed streaks as shown in Figs. 8(a), 8(c), and 8(e). Also, consistent with previous studies, the flatness factors of the three fluctuating velocity components are close to the value of 3 which Gaussian distribution bears.

E. Second-order moment statistics

Averaging (both horizontally and in time) the streamwise direction momentum equation yields $\langle \partial (\tilde{u}\tilde{w})/\partial z \rangle + \langle \partial (\tau_{xy})/\partial z \rangle = -\langle \partial \tilde{p}/\partial x \rangle$, where $\langle \tilde{u}\tilde{w} \rangle$ is the mean resolved shear stress and $\langle \tau_{xy} \rangle$ is the mean SGS shear stress. Since the simulated flow is driven by a constant pressure gradient, in the absence of viscous stresses, the normalized mean total turbulent stress grows linearly from $-1$ at the surface to 0 at the top. Because $\langle \tilde{w} \rangle = 0$, it is easy to prove that $\langle \tilde{u}\tilde{w} \rangle$ equals $\langle \tilde{u}\tilde{w}' \rangle$. Mean resolved shear stress should be negative indicating an overall tendency that faster fluid parcels moving downward ($\tilde{w}' < 0$) and slower fluid parcels moving upward ($\tilde{w}' > 0$). Figure 12 shows the vertical distribution of the mean total and partial (resolved and SGS) values of the normalized shear stress obtained from the 128$^3$ baseline simulation and the normalized SGS stresses obtained from two coarser grids (64$^3$ and 96$^3$). As expected, the coarser resolution simulations yield SGS stresses that are...
larger in magnitude than the higher resolution counterparts. The distribution of total turbulent stress is indeed consistent with the expected linear behavior. The result also serves as a confirmation of stationarity and momentum conservation of the scheme.

Figure 13 shows the vertical distribution of the variance of the resolved velocities. The current simulation results are in good agreement with the scale-dependent dynamic model results in the past work of Porté-Agel et al., which used the same numerical setup. Also, the agreement between the results from different resolution simulations is good for the two horizontal velocity components. Differences can be observed between vertical velocity variances obtained from different resolution simulations: higher resolution simulations yield higher maximum vertical velocity variances, and lower elevation where the maximum occurs. This resolution dependence is due to the fact that, near the surface, the SGS vertical velocity variance represents a relatively large fraction of the total vertical velocity variance as seen in Fig. 7. As a result, an increase in resolution leads to a smaller SGS vertical velocity variance and, in turn, a larger resolved vertical velocity variance. This contrasts with the behavior of the horizontal velocity variance, which is dominated by larger (resolved in LES) horizontal eddy scales (see also Fig. 6) and, consequently, shows little dependence on resolution.

V. SUMMARY AND CONCLUSIONS

We proposed a new nonlinear SGS model and tested it in simulations of a neutrally stratified ABL turbulence. The model uses the SGS kinetic energy to compute the magnitude of the SGS stress tensor, and the gradient tensor which can be derived by Taylor expansion of the SGS stress to determine its structure, i.e., the relative magnitude of the different tensor components. Different from standard gradient models, the formulation of the new model is derived from a class of one-equation models, which was introduced recently. Here, we use the local equilibrium hypothesis to estimate the SGS kinetic energy and adopt a clipping procedure to avoid local kinetic energy transfer from unresolved to resolved scales. This together with the fact that the model only uses local velocity gradients, and it does not require an extra filtering, make this model computationally efficient. Two approaches are considered to specify the model coefficient: a constant value of 1 and a simple correction to account for the effects of the clipping procedure on the SGS production rate.

The proposed model is examined in simulations of the well-established case of a neutral ABL flow. These simulations are the first successful calculations of ABL turbulence using an unmixed gradient scheme. In summary, the basic conclusions from this paper are: (i) the standard gradient model can be modified to achieve stable and robust simulations, (ii) the local equilibrium hypothesis together with clipping procedure may provide an estimation of the SGS kinetic energy for the model, and (iii) application to a neutral ABL flow shows the model is capable to achieve the expected logarithmic velocity profile in the near-wall region, the correct spectral scaling, as well as other important statistical characteristics of boundary layer turbulence.

It is well known that LES of the ABL is rather sensitive to the SGS model in the near-wall region. This is due to the
fact that the near-surface flow is highly anisotropic and the SGS motions account for a large fraction of the turbulence, as shown by the energy spectra of the different velocity components (Figs. 6 and 7). The proposed model shows a significant improvement with respect to other simple models, such as the standard Smagorinsky model, which is known to overestimate the nondimensional vertical gradient of the streamwise velocity near the surface and it yields energy spectra that are too steep due to its overly dissipative nature.

The model is still lacking in that, in its present formulation, it needs a priori knowledge to determine the model coefficient. It is important to note that the selected constant value is based on theoretical arguments, which are strictly only valid in the inertial subrange of high-Reynolds-number turbulence. However, the filter size usually falls outside of the inertial subrange in the near-wall region of ABL. Possible future modifications of the model include the development and testing of dynamic and scale-dependent dynamic procedures to optimize the value of the model coefficient using information of the resolved velocity field. Moreover, alternative ways of computing the SGS kinetic energy could be considered, including the solution of an additional transportation equation. A priori studies using field data could also be used to test the new closure [Eq. (1)]. Future work should also extend the implementation of a similar base model to SGS scalar fluxes.

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![FIG. 13. Vertical distribution of normalized variances of the resolved velocities obtained from (solid line) 128^3 baseline simulation, (■) 96^3 baseline simulation, and (○) 64^3 baseline simulation.](image-url)


