Three-Dimensional Buoyancy- and Shear-Induced Local Structure of the Atmospheric Boundary Layer

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ABSTRACT

Three-dimensional visualization together with statistical measures are used to describe the instantaneous local structure of the atmospheric boundary layer (ABL) under various stability states using large-eddy simulation (LES) data. To explore the relative roles of buoyancy and shear in ABL structure, a wide range of $z_i/L_{ABL}$ states, from 0.44 to 730, is analyzed. It is known that buoyancy-induced updrafts and downdrafts are primarily responsible for the upward flux of momentum, heat, and passive scalar, and strongly influence near-ground horizontal motions. These buoyancy-induced features of the convective boundary layer (CBL) are presented here in clearly observable 3D visual images of vertical velocity and temperature, showing large turbulent cell-like structure several $z_i$ in horizontal extent. The horizontal length scales of the temperature field near the ground are found to be of the order of the horizontal velocity length scales. It is noted by comparing visual structure with spectra that the disparity in the near-ground horizontal scale between temperature and vertical velocity reflects the structure of more localized thermals within the large-scale cells. By contrast, the structure of the near-neutral atmospheric boundary layer is quite different. Recent LES studies have shown that, like the flat-plate boundary layer, the dominant energy-containing motions in a near-neutral atmospheric boundary layer are near-ground shear-induced regions of high- and low-speed flow. Several features of the low-speed streaks are examined. Most importantly, there exists an influence by $z_i$-scale outer eddies on the structure of near-ground streaks, which, it is argued, strengthens at higher $z_i/L$. Warm fluid accumulates in these low-speed streaks, localizing buoyancy forces there that, at sufficiently high $z_i/L$, drive the warm fluid vertically within sheets aligned with the mean wind. These coherent sheetlike updrafts turn at the capping inversion to form the often-observed large-scale streamwise roll vortices. In this way, it is argued, shear-induced near-ground structure of the surface layer directly influences the global structure of the moderately convective ABL. It follows, therefore, that inadequacies in subgrid-scale parameterization near the ground can influence the structure of the entire ABL. In particular, the well-known overprediction of mean shear near the ground by standard Smagorinsky closures increases the streamwise coherence of the shear-induced low-speed streaks, thereby increasing the overall streamwise coherence of the vertical velocity field.

1. Introduction

Using large-eddy simulation (LES), we combine three-dimensional visualization of velocity and temperature isosurfaces with classic statistical measures to examine in detail the local instantaneous structure of the atmospheric boundary layer (ABL). From the increased understanding of large-scale 3D motions underlying the statistical structure of the ABL over a wide range of ABL states, we describe certain key dynamical processes underlying the 3D ABL motions.

The local three-dimensional structure of the atmospheric boundary layer contains buoyancy- and shear-induced motions with very different characteristic features. The structure of the buoyancy-dominated motions is relatively well understood. Field measurements (Kaimal et al. 1976; Lenschow and Stephens 1980; Wilczak and Tillman 1980; Lenschow and Stephens 1982), laboratory experiments (Willis and Deardorff 1974), and large-eddy simulation studies (Moeng 1986; Schmidt and Schumann 1989; Mason 1989) have shown that the buoyancy-induced motions tend to form concentrated regions of high magnitude positive vertical velocity fluctuation ($+w$) in “updrafts,” with compensating, relatively broad, regions of weaker negative vertical velocity fluctuation ($-w$) in “downdrafts.” These regions of dominantly upward- and downward-moving fluid, which extend throughout the boundary layer depth maintaining a strong vertical coherence, are primarily responsible for upward fluxes of momentum, heat, and passive scalar (Wyngaard and Moeng 1992) and strongly influence the near-ground horizontal velocity field (Panofsky et al. 1977; Kaimal 1978).

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A recent LES study by Moeng and Sullivan (1994) has shown that the dominant shear-induced motions in a neutral atmospheric boundary layer are streamwise streaky concentrations of low-speed (−u) motions close to the ground that align with the mean wind and are separated by less streaky high-speed (+u) motions. Low-speed “streaks” are commonly observed in smooth-surface wall-bounded shear flows (Blackwelder 1988; Robinson 1991), and there is strong evidence that low-speed streaks are a natural consequence of shear (Lee et al. 1990). In a moderately convective boundary layer, where shear and buoyancy interact, field observations (LeMone 1973; Wilczak and Tillman 1980; Lenschow and Stankov 1986) and LES studies (Sykes and Henn 1989; Moeng and Sullivan 1994) suggest that shear somehow alters the buoyancy-induced motions of the convective boundary layer (CBL) to form longitudinal roll vortices that align with the mean wind. These buoyancy-induced vertical motions influence the horizontal velocity fluctuations near the ground (Panofsky et al. 1977; Kaimal 1978).

In this LES study we use three-dimensional and two-dimensional visualization of parameter surfaces and contours (also known as isosurfaces and isocontours) to analyze the 3D structure of the primary energy containing motions in the ABL. Whereas the vertical velocity fluctuations are directly forced by buoyancy, shear tends to modulate streamwise horizontal velocity fluctuations. Under Monin–Obukhov similarity, close to the ground, the dominant energy containing vertical motions scales with the surface velocity and length scales \( u_\text{s} \) and \( z \). The horizontal motions close to the ground, however, are strongly influenced by the mixed layer eddies (downdrafts), and hence these motions tend to scale with mixed layer scales \( w_\text{s} \) and \( z \) (Panofsky et al. 1977; Kaimal 1978). A recently completed statistical study of highly resolved LES surface layer data (Khanna and Brasseur 1997) shows similar behavior and the visual structure and two-dimensional spectra presented in the current study (section 3) support these conclusions as well. However, we show here that the near-ground horizontal motions in the neutral atmospheric boundary layer are also influenced by the outer layer motions. A similar observation was also made by Höggström (1990) with field measurements.

The mechanisms underlying outer layer influence near the ground in the neutral boundary layer are not well understood. Bradshaw (1967) has suggested a non-local outer layer influence through the pressure Poisson equation. Bradshaw (1967) and Peltier et al. (1996) have shown that continuity restricts the influence of outer motions on the vertical velocity fluctuations near the ground to values of order \( z/z \), smaller than that on the horizontal velocity fluctuations. Consistent with this result, both the visualizations and the two-dimensional spectra presented here (section 3) show an obvious disparity in length scale between horizontal and vertical motions near the ground. This disparity has implications for the modeling of the lower boundary conditions for subgrid-scale fluxes in large-eddy simulations of wall-bounded flows (Wyngaard and Peltier 1996).

Although past studies (Sykes and Henn 1989; Moeng and Sullivan 1994) addressed buoyancy- versus shear-induced motions to some extent, the interactions between these two effects in moderately convective boundary layers remains to be studied in detail. For example, although the existence of large-scale longitudinal rolls in moderately convective conditions has been well documented since the early observations of Woodcock (1941) and Kuettner (1959), the criteria for their existence and the mechanisms by which they are created and which govern their scaling in a fully turbulent boundary layer are not clear. Some of the earlier analytical work based on linear stability analysis of neutral and slightly unstable planetary boundary layers did shed some light on the onset of longitudinal roll vortices. For example, Lilly (1966) and Brown (1970, 1972) analyzed the linear stability of Coriolis-induced Ekman boundary layer inflectional profiles and found that different perturbations can introduce dominant modes of instability consistent with longitudinal two-dimensional roll vortices. Asai (1970) and Kuettner (1971) analyzed the linear stability of shear with buoyancy and showed also that certain modes of instability enhance longitudinal structure at the expense of transverse structure. These and related analytical models predict the growth of the most unstable linear modes due to infinitesimal perturbation of two-dimensional mean velocity profiles. All these theories point to the existence of longitudinal structure when shear is present in the mean wind.

By contrast, LeMone (1973) considered the energetics of a fully formed three-dimensional composite roll in a fully turbulent atmospheric boundary layer by deriving a conservation equation for large-scale conditionally averaged longitudinal rolls. Various terms in the resulting energy budget were analyzed from field data. LeMone also inferred average roll height/width ratio, lateral spacing, and orientation and, by comparing her observations with the linear stability theories of Lilly and Brown, concluded that inflectional instability of the cross-stream component of the Ekman spiral plays an important role in the generation of longitudinal rolls.

Whereas theory is limited both by design and by restriction to linear predictions of what is an inherently nonlinear phenomenon, and whereas field experiments are necessarily restricted to a relatively small number of data probes, large-eddy simulation provides the full space–time evolution of the larger-scale motions within the atmospheric boundary layer—information inaccessible with any other technique. In this study we use LES to analyze the systematic changes in large-scale atmospheric structure associated with systematic changes in atmospheric stability state. By analyzing the full range of stability states, from near neutral to highly convective, and by placing this analysis in context with knowledge of buoyancy- and shear-driven turbulence within
Table 1. Details of the ABL states analyzed, created from 128³ large-eddy simulation. Here, $L$, $L_*$, and $L_z$ are the streamwise, cross-stream, and vertical dimensions, respectively, of the computational domain. Also, $Q_i$ is the average surface temperature flux, $U_i$ is the geostrophic wind velocity, $z_i$ is the boundary layer depth (height of minimum vertical temperature flux), $u_z$ is the surface friction velocity, $L$ is the Monin-Obukhov length scale, $w_i$ is the mixed layer convective velocity scale, $\Delta_z$ is the interfacial layer thickness (region of negative vertical temperature flux), $\Delta \Theta$ is the mean potential temperature jump across the interfacial layer.

<table>
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<th>$-z_i/L$</th>
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<th>3</th>
<th>8</th>
<th>65</th>
<th>730</th>
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<td>$L'(km)$</td>
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<td>6</td>
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</table>

both the geophysical and engineering communities, we develop arguments for the formation of large-scale longitudinal rolls in the moderately convective ABL. We argue that the upward leg of these horizontal roll vortices originates in the near-ground low-speed streaks that result from shear. Our LES-based analysis suggests that it is in the transfer of information by convective motions from the lower shear-dominated ABL to the upper buoyancy-dominated ABL that lies the key to the generation, structure, and prediction of longitudinal rolls.

A detailed discussion on shear-induced streaks and the formation of sheetlike updrafts is given in section 3 and a related discussion of local structure in temperature follows in section 4. In section 5 we discuss the relative contributions of vertical and horizontal motions to the upward flux of heat and momentum using conditional statistics. We end in section 6 with a discussion of subgrid scale (SGS) parameterization effects on large-scale structure in the moderately convective ABL.

2. The large-eddy simulations

The atmospheric boundary layer was simulated over a wide range of stability states (0.44 $\leq -z_i/L \leq$ 730) using Moeng’s LES algorithm (Moeng 1984) on 128³ grids over a computational domain approximately twice the capping inversion depth ($z_i$) in the vertical and five or six $z_i$ in the horizontal. The global parameters of the five ABL states analyzed are given in Table 1. We applied the modified Smagorinsky subgrid-scale parameterization proposed by Sullivan et al. (1994), which was designed to reduce overpredictions of mean shear in the surface layer of a near-neutral ABL by standard Smagorinsky closures. We compare this closure with a more standard Smagorinsky closure (Moeng 1984) in section 6 to evaluate the role of SGS closure in predicting ABL structure. Details of the algorithm and numerical simulations are given in Khanna and Brasseur (1997).

3. Velocity field induced by buoyancy and shear

We characterize the dominant energy-containing motions as regions in the boundary layer where a fluctuating turbulent kinetic energy (TKE) component is locally large and contributes significantly to the component velocity variance. Such regions are expected to be spatially and temporally coherent over length scales and timescales of order of the integral scale and eddy turnover time, respectively, and are expected to make significant contributions to turbulent momentum and temperature fluxes. The primary sources of turbulent kinetic energy in the unstable atmospheric boundary layer are buoyant production from vertical turbulent temperature flux and shear production from the interaction of vertical turbulent momentum flux with mean shear.

The component turbulent energies for a horizontally homogeneous boundary layer are governed by

$$\frac{1}{2} \frac{\partial \omega_u \omega_u}{\partial t} = - \frac{\partial U_i}{\partial x_i} \frac{\partial U_i}{\partial x_i} - \frac{1}{2} \frac{\partial U_i \omega_u \omega_u}{\partial x_i} - \frac{1}{\rho_0} \frac{\partial P}{\partial x_i} \delta_{ij}$$

$$+ \frac{\rho_0 \frac{\partial u_u}{\partial x_i}}{T_0} \frac{\theta}{\delta_{ij}} - \varepsilon_{ij} \Omega \omega_u \omega_u$$

with no summation on Greek indices ($i, j, k = 1, 2, 3$). Here $u_u$, $\theta$, and $p$ are fluctuating velocity, temperature, and pressure; $U_u$ is mean velocity; and $\Omega$ is the earth’s angular velocity. The horizontal coordinates $x_i$ are chosen aligned with the mean wind at each $x_i$. Note that whereas buoyant production ($g/T \omega \theta$) adds energy directly to vertical motions on average, shear production ($-\frac{\partial w_i}{\partial z} U_i \partial z$) adds energy directly to horizontal turbulent motions. Pressure strain-rate correlations (fourth term on rhs), then redistributes the turbulent energy among the three velocity components. Consequently, the strongest buoyancy-induced motions are in the vertical velocity component, while the strongest shear-induced motions are in the streamwise velocity component. We analyze here the three-dimensional structure of the vertical and streamwise velocity components—first for buoyancy- and shear-dominated boundary layer states and then for intermediate states where buoyancy and shear interact in determining large-scale ABL structure.

a. The purely convective boundary layer

1) Vertical velocity

The vertical velocity field in the highly convective state is well understood. Field measurements (Kaimal et al. 1976; Lenschow and Stephens 1980; Wilczak and Tillman 1980) indicate that the buoyancy-induced ver-
tical velocity field is characterized by regions of intense upward motions, or updrafts, and compensating regions of less intense downward motions, downdrafts. Updrafts originate as small-scale thermal plumes near the ground that grow in horizontal scale with distance from the ground and merge with neighboring plumes to form larger-scale regions of upward-moving warmer fluid in the mixed layer. The updrafts are separated by broader regions of gentler downward-moving cooler fluid. In the mixed layer the characteristic dimensions and spacing of the updrafts scale with the boundary layer depth \( z_i \) (Kaimal et al. 1976). The updraft regions make a significantly larger contribution to the vertical flux of heat and momentum than do the downdraft regions (Wyngaard and Moeng 1992). Our LES studies are consistent with those of Schmidt and Schumann (1989) and Mason (1989), where the updrafts in the simulated purely convective boundary layer form a large-scale turbulent cellular pattern similar to that observed in turbulent Rayleigh–Benard convection.

The growth and merger of plumes near the ground to form larger-scale plumes are reflected in a roughly linear increase in horizontal integral length scale of vertical motions with distance from the ground within the surface layer. Field measurements in the highly convective state (Kaimal et al. 1976) indicate that the peak in the vertical velocity spectrum moves to lower wavenumbers with increasing distance from the ground with the corresponding length scale increasing roughly linearly up to \( z_i / \approx 0.1 \).

In Fig. 1 we show two-dimensional horizontal spectra of...
vertical and streamwise velocity and temperature at four heights from the ground in the simulated highly convective ABL state \((-z_i/L = 730\)). The two-dimensional spectrum is obtained by integrating the 2D spectral density function over circular rings of constant \(k = \sqrt{k_x^2 + k_y^2}\). Consistent with the observations of Kaimal et al. (1976), the peak in \(w\) spectra \(\langle k_w \rangle\) moves to lower wavenumbers with increasing distance from the ground. Note that Fig. 1 indicates that, for this buoyancy-driven state, \(\langle k_w \rangle = z\) for \(z/z_i \leq 0.25\).

The horizontal scales of vertical velocity are characterized by the integral scales

\[
l_{w}(z) = \int_{0}^{\infty} \frac{r_{w}}{R_{w}(0,z)} dr_{w},
\]

where

\[
R_{w}(r_{w},z) = u_{w}(x_{r})u_{w}(x_{r} + r_{w}).
\]

Here, \(r_{w}\) is a two-point horizontal separation vector and the ensemble average is replaced by area averaging on \(x_{r}\) over horizontal planes. Lenschow and Stankov (1986), who measured two-point correlations of vertical velocity in the convective boundary layer over ocean and land surfaces, found that the ratio of streamwise to cross-stream integral length scales \(l_{w}/l_{ww} = 1.7\) for \(-z_i/L \approx 8–55\). As discussed in section 3c, we find this elongation in the streamwise direction to be an effect of shear. Lenschow and Stankov fitted ensemble averaged streamwise \((x')\) and cross-stream \((y')\) length scales to

\[
\frac{l_{w}}{z_i} = \frac{l_{ww}}{2z_i} = 0.24 \left( \frac{z}{z_i} \right)^{1/2}.
\]

In Fig. 2 we plot \(l_{w}/z_i\) and the ratio \(l_{ww}/l_{w}\), obtained from LES together with equation (4) for \(-z_i/L \geq 0.44\) to 730. In the near-neutral and moderately convective cases, which are shown in Fig. 2 for comparison with the highly convective case and later references in sections 3b(2) and 3c, we chose the \(x'\) axis to be aligned with the direction of elongation of the vertical velocity field. To determine this direction we calculate the horizontal integral length scales of \(w\) at different angles to the direction of the imposed geostrophic wind (our \(x\) axis) on the horizontal plane midway through the ABL \((z = z/2)\) and identify the angle where the integral scale is maximum. Figure 2 gives the streamwise and cross-stream integral scales, along and perpendicular to the direction of elongation, as a function of \(z/z_i\). Because the disparity between streamwise and cross-stream integral length scales is a consequence of shear, the ratio of the two length scales depends both on \(z/z_i\) and \(z_i/L\). However, the average of the streamwise and cross-stream length scales \((l_{w})\) is much less sensitive to \(z_i/L\) near the ground and agrees reasonably well with Eq. (4), especially for the highly convective case. The LES prediction in Fig. 2a, showing a decrease in \(l_{w}\) above \(z_i/L \approx 0.7\), is consistent with the measurements of Caughey and Palmer (1979) but inconsistent with measurements of Kaimal et al. (1976) and Lenschow and Stankov, which suggest continuous growth up to \(z_i\). However, as argued by Carruthers and Hunt (1986), the variation in characteristic scale near the capping inversion is related to the stability of the overlying stably stratified layer. A strong capping inversion, such as used in LES, forces a reduction in the characteristic length scale approaching the capping inversion.

Figure 3 shows a three-dimensional surface of positive vertical velocity in the CBL from two views: from the side (upper panel) and from above (lower panel). The surface identifies concentrated regions of large upward vertical velocity fluctuations. Note from the side view that smaller plumes originating near the ground grow and merge with neighboring plumes to form \(z_i\)-scale updrafts with strong vertical coherence. The lower panel shows that these \(z_i\)-scale plumes form larger cel-
lular patterns with characteristic length scale that also scales on $z_i$.

Details of upward and downward vertical velocity structure are more clearly observed in Fig. 4, which displays contours of $w$ on horizontal ($x$-$y$) planes at different heights $z/z_i$. On average, the width of concentrated updraft and downdraft regions grows with distance from the ground, while the large cellular structure formed by the concentrated updrafts persists through the boundary layer with fixed scale. The updraft regions are stronger, more concentrated, and more spatially coherent than the downdraft regions. This is especially apparent away from the ground where well-defined large-scale cellular patterns of concentrated updraft regions surround much broader and weaker downdraft regions.

Figure 5 shows contours of vertical velocity on ver-

**Fig. 3.** Three-dimensional surface of $w = +1.5w^*_i$; $-z_i/L = 730$. The domain shown is 5 km ($x$) by 5 km ($y$) by 1 km ($z$); top panel: cross-stream view; bottom panel: angled view of ABL from the top.
tical planes showing the strong vertical coherence of the updrafts and downdrafts. The upper figure was chosen to cut through an updraft region and the lower figure to show a cross-sectional cut through a Rayleigh–Bénard cell. The lower figure shows that the broader downdraft regions are between the updrafts and that the edges of the thermals are marked by strong horizontal gradients in vertical velocity. Some small rather weak plumes near the ground are suppressed by stronger downdrafts, while other plumes near the ground merge with their neighbors to form larger stronger updrafts. Similarly, at the capping inversion, where upward-moving fluid is forced to turn downward, some small-scale downdrafts are suppressed by larger stronger updrafts.

To extract from the vertical velocity field the largest-scale motions that scale on $z$, the vertical velocity field was filtered in the horizontal plane using a circularly symmetric Gaussian filter in horizontal wavenumber $k$,

$$g(k) = G(k_p) e^{-6(k_p - k)^2/\Delta^2},$$

where $G^2(k_p) = E^2(k_p)$, see Fig. 1, is the 2D variance spectrum of $w$ at $k = k_p$, and $\Delta = \Delta(k_p)$ is the filter width. Based on Fig. 1, the integral-scale motions of the vertical velocity is filtered by choosing $k_p = z^{-1}$. To better capture smaller-scale detail close to the ground, the filter width increases with $k_p$ like $\Delta = 10 \ln((L_x/2\pi)k_p)$, where $L_x$ is the streamwise extent of the computational domain. The filtered velocity field is the
two-dimensional inverse Fourier transform of $g(\kappa)\tilde{w}(\kappa)$, where $\tilde{w}(\kappa)$ is the horizontal Fourier coefficient of vertical velocity. Figure 6 shows three-dimensional surfaces of unfiltered $w$ (light–solid) overlaid with filtered $w$ (dark–mesh). Note that the largest integral-scale motions identify the Rayleigh–Benard updraft regions, implying that smaller-scale motions account for the localized thermals within the largest-scale cellular structure.

2) Horizontal velocity

In a purely convective boundary layer the horizontal fluctuations receive energy, on average, from the vertical velocity through the pressure strain-rate intercomponent energy transfer term in Eq. (1). Apparently, then, this term is large near the ground where field measurements (Papoffsky et al. 1977; Kaimal 1978) indicate that large-scale downdrafts create horizontal sweeping motions, producing horizontal fluctuations that scale on the mixed layer scales $w^*$ and $z_i$. Note in Fig. 1, for example, that the two-dimensional horizontal spectrum in the CBL peaks at the same wavenumber at all $z/z_i$, while the peak in the $w$ spectrum scales on $z^{-1}$ up to the mixed layer where both vertical and horizontal spectra peak at nearly the same scale. These results are in good agreement with the field observations of Kaimal (1978), which show a large disparity in length scale between horizontal and vertical fluctuations in the surface layer, a peak in the streamwise velocity spectrum that scales on $z_i$ at all $z$, and a peak in the vertical velocity spectrum that scales on $z$ in the surface layer and on $z_i$ in the mixed layer.

Three-dimensional constant energy surfaces surrounding regions of concentrated horizontal kinetic energy are shown in Fig. 7. The most intense fluctuations are near the ground where the convective downdrafts are turned to the horizontal direction. These regions of horizontal fluctuation tend to lie between the thermals, are visibly less coherent than the updraft regions, and occupy a much broader horizontal region than do the updrafts. Intense horizontal motions are also observed near the capping inversion where updrafts are also turned to the horizontal direction.

b. The neutral boundary layer

1) Horizontal velocity

Coherent streamwise elongated “streaks” of lower-than-average streamwise velocity are ubiquitous in turbulent shear flows and have been observed in a variety of contexts. Since the early observations of Kline et al. (1967), decades of research on these ubiquitous streaks have shown their existence in all wall-bounded shear flows, as well summarized by Robinson (1991). Robinson and other researchers in the engineering community have shown that the near-wall streaks are kinematically tied to the presence of streamwise counter-
rotating vortices; streaks of slow-moving fluid are formed along the upward-moving convergence regions between the vortices. An important analysis by Lee et al. (1990) in shear flow turbulence without a wall showed that streaks, and the corresponding streamwise counterrotating vortices, are a direct consequence of shear acting on an underlying turbulence field of velocity fluctuations. Thus, streaks are directly related to the existence of shear and only indirectly to the presence of a surface (which creates the shear). The greater the shear (appropriately normalized by the large-eddy timescale), the more elongated are the streaks.

Robinson found that concentrations of low-speed streamwise fluctuations ($u$) in the flat-plate boundary layer are much more elongated than the high-speed regions and that, although some low-speed streaks ap-
pear to extend over much of the boundary layer depth, streaks in the lower part of the low Reynolds number boundary layer are much more apparent. Compared to the near-wall region, in the outer regions of the boundary layer \( u \) fluctuations were found to be concentrated in spanwise-alternating regions of concentrated \( +u \) and \( -u \) with streamwise length scales of order the boundary layer thickness and average spanwise width larger than near-wall streaks.

The structure of the high Reynolds number flat-plate boundary layer (FPBL) outside the viscous sub-layer is related to the neutral ABL. The primary feature of the streamwise motions, the low-speed streaks, are also observed in the near-neutral atmospheric boundary layer (Deardorff 1972; Moeng and Sullivan 1994).

In LES of the near-neutral boundary layer, the ground is modeled as a rough surface (roughness...
height \( z_s \approx 1 \text{ cm} \) with no viscous or buffer layer. Nevertheless, prominent streaks of low-speed flow are observed close to the ground in regions of high shear consistent with direct numerical simulation (DNS) of homogeneous shear-flow turbulence (Lee et al. 1990). Consistent with the observations, Fig. 8 shows contours of streamwise velocity on horizontal planes at various heights in the near-neutral ABL \((-z/L = 0.44\)). Elongated concentrations of high- and low-speed fluctuating streamwise velocity are evident throughout the boundary layer, particularly near the ground. The low-speed regions are clearly much more elongated than are the high-speed regions. Those low-speed streaks that persist to the mid boundary layer grow in spanwise scale and diminish in intensity. The intensity of the high-speed regions \((u > 0\), however, decreases more rapidly with height than does the intensity of the low-speed streaks \((u < 0\), as shown in Fig. 9 where the skewness of \(u\) is plotted against \(z/z_i\). With the exception of a very narrow region adjacent to the ground, skewness is negative, indicating a predominance of negative \(u\) fluctuations that, from Fig. 8, are concentrated in streamwise coherent highly elongated streaks.

Figure 10 shows horizontal spectra of the velocity component and temperature variance at different heights
$z_i$ in the near-neutral ABL. Note that, as with the CBL (Fig. 1), the peak in the vertical velocity variance spectrum is given by $\kappa_v = z^{-1}$ when $z/z_i \leq 0.2$, roughly. Also as with the CBL, the peak in the streamwise velocity variance spectrum is at scales $z_p$ much larger than $z$ and is independent of $z$.

Figure 11 shows contours of the streamwise velocity fluctuations along both streamwise and lateral vertical planes. The upper figure of the cross-stream plane indicates the persistence of two to three low-speed regions to the capping inversion over the 3-km span of the figure. The streamwise vertical plane of the lower figure shows clearly the vertical coherence of one of the streaks. Note from Fig. 8 that the average number of streaks per unit span decreases with $z$ from perhaps six to seven near the ground to only two to three in the mid boundary layer across the span of computational domain (3 km). Figure 12 shows the average streak spacing $\sigma$ as a function of height, where average streak spacing is calculated by choosing a negative threshold for $u$ and averaging the spanwise distances between neighboring negative peaks over horizontal planes. Whereas close to the ground $\sigma = 0.5z_i$, streak spacing increases at higher $z/z_i$, suggesting the persistence of only a few streaks in the mid to upper boundary layer. Figure 11 shows that the large average streak spacing in the outer boundary layer is a consequence not of the growth and amalgamation of streaks with $z$, but rather a vertical coherence of a subset of streaks from the ground through the boundary layer.

Figures 12 and 11 indicate that two scales characterize the streamwise fluctuating velocity in the neutral ABL—a local scale set, presumably, by mean shear and $z$, underlies fluctuations near the ground, and the outer layer scale $z_i$, characterizing a subset of streamwise turbulent motions with strong vertical coherence. This subset of $z_i$-scaled streaks connects the lower and upper atmospheric boundary layer. We shall argue that this coupling between near-ground and global ABL structure strengthens at higher $z_i/L$ (section 3c).

2) Vertical velocity

Robinson (1991) observed in low Reynolds number DNS of the flat plate boundary layer that three-dimensional regions of high-intensity $-u$ and $+w$ fluctuations, and $+u$ and $-w$ fluctuations have a strong spatial correlation. Near the wall, high-intensity $+w$ regions were found to contain a streaky topography like $u$, but with an average streamwise dimension much smaller than the $-u$ streaks. Although the variance of $w$ is much smaller than $u$ near the wall, Robinson found that along near-wall low-speed $u$ streaks, small-scale localized regions of intense $w$ activity could be found. In the outer layer, by contrast, the characteristic scale of $w$ motions approaches the scale of $u$ motions, and the overlap between the two fields gives rise to large-scale regions of negative $u$ fluctuations.

LES of a near-neutral ABL shares some similarities with the low Reynolds number FPBL. Figure 13 shows a three-dimensional surface of negative $u$ in dark together with a surface of positive $w$ in light. Note that localized pockets of concentrated vertical velocity emerge and extend vertically through the boundary layer from near-ground low-speed streaks. Although these lower intensity regions of concentrated vertical velocity are spatially correlated with the low-speed streaks, the streamwise coherence length of the intense $+w$ regions is clearly much smaller than the streamwise length scale of negative $u$ fluctuations.

To see the structural relationship between $w$ and $u$ fluctuations more clearly, compare the pattern of $w$ contours in Fig. 14 with the pattern of $u$ contours in Fig. 8. Close to the ground, the $+w$ fluctuations are much smaller in horizontal scale than the $-u$ streaks. The scale of vertical velocity is observed to increase with $z$ to mid ABL where a strong spatial correlation is observed between regions of concentrated $u < 0$ (Fig. 8) and $w > 0$ (Fig. 14). We conclude that in the outer neutral boundary layer vertical motions are spatially correlated with horizontal motions providing a mechanism by which outer $z_i$-scale motions communicate with the ground.

The average horizontal integral length scale of vertical velocity fluctuations $l_w$ and the ratio of streamwise to cross-stream scales $l_w/l_{uw}$ are plotted in Fig. 2 (curve 1). Whereas the average integral scale $l_w$ grows rapidly with $z$, peaking near the mid boundary layer, the aspect ratio of the vertical velocity fluctuations is approximately 5 up to the mid boundary layer, indicating that even though the highest intensity vertical motions are rather small in streamwise extent, on average the $w$ fluctuations are elongated in $x$ near the ground.

The rapid growth in vertical velocity length scale with $z$ is also apparent in the spectra of Fig. 10, as is the
disparity between the $w$ and $u$ horizontal scales. Note that at higher $z$ the $w$ spectral peak approaches the $u$ spectral peak consistent with the conclusion obtained visually by comparing the contours of Figs. 14 and 8.

c. Moderately convective boundary layers

Field measurements (LeMone 1973) have shown the existence of horizontal roll vortices in moderately convective boundary layers that align with the mean wind. Sykes and Henn (1989) observed roll structures in their large-eddy simulations when $-z_i/L < 10$, while Moeng and Sullivan (1994) observed these structures in LES for $-z_i/L > 1.5$. Whereas the cross-stream spacing of the rolls appears to scale with the boundary layer depth and their streamwise extent appears to be several $z_i$, the mechanisms underlying the structure and scaling of the rolls have not been fully elucidated.

We observe clear roll vortices in our 128$^3$ simulations of the ABL at the $-z_i/L = 3$ and $-z_i/L = 8$ stability states. The rolls are visually prominent in Fig. 15 where the three-dimensional surface of vertical velocity fluctuation in the $-z_i/L = 8$ state is shown. The two elongated regions of concentrated updraft at this level are spaced about $2z_i$ in the cross-stream direction. The upper figure, looking cross stream through the boundary layer, shows that close to the ground updrafts form as small-scale plumes that grow with distance from the ground and merge with neighboring plumes in the streamwise direction. The streamwise-coherent sheets of updraft extend vertically through the boundary layer depth.
Interestingly, the sheet-like updrafts in Fig. 15 appear to extend throughout the horizontal computational domain, casting doubt on the adequacy of our domain size to accurately predict the streamwise integral length scale of $w$ shown in Fig. 2. Figure 16 shows the streamwise ($x'$) autocorrelation function, $R_{ww}(x', z)$ [see Eq. (3)], at $z = z_i/2$ for the moderately convective case ($-z_i/L = 8$). The $x'$ axis is taken to be the one for which the streamwise integral length scale obtained by integrating $R_{ww}(x', z)$ [Eq. (2)] is maximum, presumably along the roll orientation. The function does not drop to 0 for large separation distances, as one would ideally expect. Instead, it reaches an asymptotic value close to 0.1. Our computational domain does appear to underestimate the streamwise integral length scales, especially for the moderately convective case (curve 2). Nevertheless, the length scales computed from our data do provide a qualitative picture of streamwise elongation of roll vortices and are useful supplements to the visual images. The curves for near-neutral and highly convective cases (curves 1, 3, and 4), however, are quantitatively accurate.

The roll structure of the turbulent velocity is more explicit in the contours of $w$ in Fig. 17. The cross-stream ($y-z$) plane (upper figure) shows strong narrow buoyancy-induced updrafts in red surrounded by broader and less intense downdrafts. The roughly streamwise ($x-z$) plane in the lower figure together with Fig. 15 suggests streamwise coherence within the updrafts extending over scales of order $3z_i$. The horizontally anisotropic structure of the horizontal roll vortices apparent in Figs. 15 and 17 is shown quantitatively in Fig. 2b (curve 2) by the ratio of streamwise to cross-stream integral
scales. Note that the length scale ratio is largest near to the ground in a region extending to about $0.2z_i$ and decreases to nearly one at the capping inversion.

Because buoyancy effects are horizontally isotropic, the transition from the large-scale Rayleigh–Benard cell-like structure of Fig. 3 to the large-scale horizontal roll structure of Fig. 15 must be related to the existence of shear in the mean wind. We now argue that the origin of the streamwise and vertically coherent updrafts observed in Fig. 15 and 17 is a direct consequence of the formation of low-speed streaks [discussed in section 3b(1)] by mean shear near the ground, where mean shear is maximal.

From the first recognition by Kline et al. (1967) that streaks observed with passive markers are, in fact, the same streaks defined by negative turbulent velocity fluctuations, it has been observed that scalar has a strong tendency to concentrate within the streaks. Indeed, many measurements, both in the laboratory and on the computer, have shown that fluctuating passive scalar is very
strongly correlated with fluctuating streamwise velocity near the wall in wall-bounded shear flows. More recently, with the availability of direct numerical simulation, it has been shown that this correlation is a result of a strong spatial overlap between coherent regions of large scalar fluctuation and negative velocity fluctuation (e.g., see Horiuti 1988 and Kim 1988).

Regions of high positive fluctuating scalar are found in regions of low negative fluctuating streamwise velocity when scalar moves, on average, from the wall into the turbulent flow, and regions of low fluctuating passive scalar are found in regions of low negative fluctuating streamwise velocity when scalar moves, on average, to the wall from the turbulent flow. The concentration of fluctuating passive scalar of one sign or the other in the low-speed streaks can be understood by considering the movement of fluid particles from the wall, from low to high mean velocity regions, between the counterrotating vortices. If mean scalar is larger at the wall, a fluid particle moving away from the surface will tend to have lower than average velocity with higher than average scalar, and vice versa for a particle moving toward the surface.

Since temperature is like a passive scalar at low $-z_i/L$ (near neutral), warm fluid has a strong tendency to concentrate in the low-speed streamwise streaks. We
like to emphasize that the formation of streamwise streaky regions of low-speed ($-u$) flow and the concentration of temperature in these streaky regions, as observed by Horiuti (1988) and Kim (1988) in neutral flat-plate boundary layers, is purely a consequence of shear.

Like other wall-bounded shear flows, in moderately convective atmospheric boundary layers vertical temperature flux exists at the ground in the presence of strong mean shear. Consequently, high positive temperature fluctuations tend to concentrate in shear-induced low-speed streaks near the ground. However, unlike passive temperature fluctuations in the neutral ABL, at higher $-z_i/L$ the concentration of warm fluid in the streaks increases buoyancy forces there, tending to drive the fluid upward. If buoyancy is sufficiently strong, local
buoyancy-induced plumes are formed in the streaks that grow and merge with other plumes along the streak, creating streamwise coherent sheets of warm upward-moving fluid. On reaching the capping inversion, the upward-moving fluid is forced to turn and form the downward legs of horizontal rolls. These downdrafts would tend to reduce or suppress the coherence of weaker updrafts emerging from neighboring streaks. We argue that a feedback loop is established whereby weaker buoyancy-driven flow in some low-speed high-temperature streaks is continually suppressed by strengthening buoyancy-driven thermals that communicate with the capping inversion. Consequently, the equilibrium state consists of coherent sheetlike updrafts emerging from near-ground low-speed streaks that scale on $z_i$.

By this argument, at lower $-z_i/L$ one might expect to find more evidence of streaks close to the ground that do not scale on $z_i$. At low enough $-z_i/L$, buoyancy forces would be insufficient to drive large streamwise coherent vertical motions, and the vertical velocity field will concentrate instead in the weak small-scale structures of Fig. 13. On the other hand, at large $-z_i/L$ shear is too weak to organize the streamwise velocity into well-defined low-speed streaks. Temperature no longer preferentially concentrates within elongated streamwise coherent structures, and the buoyancy-driven thermals form the natural Rayleigh–Benard cellular structure of Figs. 3 and 4.

Figure 18 shows contours of streamwise fluctuations ($u'$) on horizontal planes in the moderately convective ($-z_i/L = 8$) ABL state. Although the coherence in the streamwise direction is not as strong as in the near-neutral state of Fig. 8, well-defined elongated regions of low-speed fluid (blue) extend through the surface layer into the mixed layer (note that the mean wind in
Fig. 18 is roughly 20° relative to $x$). We argue that this reduced coherence in the low-speed regions near the ground is a consequence of downdrafts that strongly influence the horizontal fluctuations there. Nevertheless, low-speed shear-induced streaks are apparent in the $-z_i/L = 8$ state.

Figures 19 and 20 show contours of temperature and vertical velocity fluctuations on the same horizontal planes as in Fig. 18. Note from Fig. 19 that close to the ground, concentrations of high temperature tend to align with the low-speed streaks of Fig. 18 and that the characteristic scale of the $\theta$ streaks is close to the characteristic scale of the $u$ streaks. This will be discussed further in section 4. Figure 20 shows that low-speed high-temperature streaks are also regions of high vertical velocity. Near the ground vertical velocity tends to concentrate in structures narrower than the concentrations of $-u$ and $+\theta$.

Note from Figs. 19 and 20 that the intensity of vertical velocity fluctuations decreases rapidly at the ground where temperature variance is large, and vice versa. Near the ground local pockets of intense $+w$ occur along low-speed streaks, while away from the ground $+w$ concentrates in broader regions overlapping with broader concentrations of low-speed horizontal flow. This observation indicates that the buoyancy-induced plumes
emerge along the low-speed streaks near the ground and merge with neighboring plumes in the streamwise direction. Merging of plumes in the spanwise direction is not observed, apparently because the spanwise streak spacing is much larger than the plume width.

Two-dimensional spectra of velocity and temperature variance are shown in Fig. 21 for $-z_i/L = 8$ state. Note that whereas close to the ground a disparity in length scale is apparent between the $u$ and $w$ spectra, this disparity disappears farther from the ground, consistent with the visual comparisons between Figs. 18 and 20.

To show more clearly the emergence of sheetlike updrafts from near-wall low-speed streaks and the suppression of some near-wall thermals by strong downdrafts, we show in Fig. 22 contours of $u$ (a), $w$ (b), and combined $u-w$ contours on the cross-stream plane. Note, in particular, the correlation between streaks of low-speed streamwise fluctuations and sheetlike updrafts of vertical velocity fluctuations, shown clearly in the bottom figure. Consistent with the quantified streak spacing shown in Fig. 12, the top figure suggests that the average streak spacing in the middle of the boundary layer is roughly constant and of order of the boundary layer depth.

4. Temperature field structure

Temperature fluctuations tend to be large in regions of large heat flux at the ground and in the entrainment-
dominated capping inversion. Because high temperatures near the ground drive the buoyant plumes (+w) that extend across the ABL, there exists a strong correlation between the temperature and the vertical velocity field in an unstable boundary layer. These updrafts are blocked by the capping inversion, where vertical motions turn to the horizontal. By contrast, in the near-neutral boundary layer, temperature is a passive scalar with its three-dimensional structure reflecting shear-dominated motions.

Figure 23 shows three-dimensional isosurfaces of temperature fluctuations (dark) and vertical velocity fluctuations (light) in the fully convective ABL (−z/L = 730). The most intense temperature fluctuations occur near the ground and at the capping inversion. Note that the updrafts emerge from local regions of high temperature near the ground, but they attain maximum vertical momentum near the middle of the boundary layer where temperature fluctuations are low. Figure 24 shows contours of the temperature field on horizontal planes for comparison with the vertical velocity contours of Fig. 4. As in the case of vertical velocity, high-temperature regions form a cellular pattern at the same horizontal scale. However, near the ground the average scale of localized temperature plumes within the Rayleigh–Benard cellular structure is significantly larger.
than the localized vertical velocity plumes at the same height, explaining the disparity in scale apparent in the horizontal spectra of temperature and vertical velocity in Fig. 1 (near the ground the temperature spectra peak at wavenumbers significantly lower than the peak in \( \omega \) spectrum).

As discussed in the previous section, in a moderately convective boundary layer high-temperature fluid tends to concentrate in the shear-induced low-speed streaks. We argued that this correlation between high temperature and low horizontal velocity is the source of the strongly anisotropic sheetlike updrafts and horizontal roll vortices shown visually in Figs. 15 and 17. It was also argued visually (Figs. 18 and 19) that the characteristic length scale of \( +\theta \) streaks is of order the characteristic scale of \( -u \) streaks. Note that, consistent with this visual observation, the temperature and horizontal velocity spectra in Fig. 21 peak at nearly the same wavenumber. The \( \omega \) spectra, by contrast, peak at high wavenumbers near the ground (\( \kappa^\omega \approx z^{-1} \)), consistent with a visually apparent difference in scale between localized concentrations of temperature and vertical velocity along the low-speed streaks (Figs. 18–20). Figures 18 and 19 indicate that the correlation between high temperature and low streamwise velocity persists to the midABL.

In the near-neutral boundary layer, temperature acts as a passive scalar and buoyancy forces are insignificant. Figure 25 shows horizontal contours of temperature along horizontal planes for comparison with same \( u \) contours of Fig. 8 (\( -z/L = 0.44 \)). Note that, like the flat-plate boundary layer, higher temperature fluctuations are highly correlated with the near-wall low-speed streaks.
5. Structure of the fluxes

In horizontally homogeneous and quasi-steady barotropic boundary layers, ensemble averaged fluxes of momentum, heat, and passive scalar vary linearly from their ground values to their respective entrainment values at the capping inversion (Wyngaard 1992). Although the energy-containing motions are the primary contributors to these fluxes, the relative contributions from updrafts and downdrafts (Wyngaard and Moeng 1992) and from low-speed and high-speed horizontal motions are very different. These relative contributions are analyzed in this section.

Figure 26 shows conditional probability density functions (pdf) of fluctuating temperature flux \( w\theta \) conditioned on \( w \) together with pdfs of \( w \) at various heights in the highly convective boundary layer \( (-z/L = 730) \). The conditional pdf is defined as the expected value of \( w\theta \) for \( w \) in the range \( w \pm \Delta w \). Vertical velocity fluctuations in a convective boundary layer are positively skewed throughout the boundary layer depth (Hunt et al. 1988). Positive skewness is also apparent in the pdfs of \( w \) in Fig. 26. Note from the conditional temperature flux that vertical flux is dominated by upward vertical motions throughout the ABL. This asymmetry between upward and downward motions in contributing to temperature flux increases with \( z \) and is strongest near the middle of the boundary layer where nearly all vertical flux is in the upward motions.

The structure of the relationship between vertical flux and velocity is shown in Fig. 27 where three-dimensional isosurfaces of positive \( w \) (light-mesh) and positive \( w\theta \) (dark-solid) are displayed together. Note that the regions of strong updraft are also the regions of strong vertical temperature flux throughout the boundary layer depth, except near the capping inversion where the penetrating updrafts enter a region of warmer stably stratified fluid. At the capping inversion the updrafts are at lower temperature relative to their surroundings, causing a local change in the sign of the temperature flux.

For comparison with the highly convective ABL of Fig. 26, Fig. 28 shows the conditional pdf of \( w\theta \) for the moderately convective ABL \( (-z/L = 8) \). Whereas the asymmetry between updrafts and downdrafts continues to be strong and the updrafts remain the primary source to vertical temperature flux, the strongest asymmetry occurs at lower heights \( (\approx 0.25z_c) \) than the CBL \( (\approx 0.5z_c) \).

The updrafts are also the major contributors to mo-
mentum flux, but the disparity is not as strong as with temperature flux. Figure 29 shows conditional pdfs of $uw$ conditioned again on $w$ for $-z/L = 8$. Note that, whereas the momentum flux is positively skewed like temperature flux, unlike temperature flux the momentum flux in upward- versus downward-moving fluid is nearly the same close to the ground. Farther from the ground, however, the updrafts dominate the momentum flux. Interestingly, in the middle of the boundary layer the strongest downdrafts contribute positively to momentum flux, suggesting that large negative $w$ is correlated with negative $u$. However, the net contribution of downdrafts to the local flux is actually negative due to the dominant contribution from gentler downdrafts, which contribute negatively to the local flux.

The mechanisms driving the momentum and tem-
Fig. 24. Contours of $\theta$ on horizontal planes at different $z/L$; $-z/L = 730$; $\theta_* = Q_0/w_*$.  

Temperature flux in a neutral ABL are very different from those in a convective boundary layer. Whereas flux is carried primarily by buoyancy-induced vertical motions in convective and moderately convective boundary layers, in the neutral boundary layer the upward fluxes of momentum and passive scalar are a consequence of shear-induced motions directly related to concentrations of high- and low-speed streamwise velocity (streaks). To quantify the relationship between streamwise velocity and vertical flux, we show in Fig. 30 the pdf of $uw$ conditioned on $u$ at various heights in the near-neutral boundary layer ($-z/L = 0.44$). We observe that whereas close to the ground the high- and low-speed regions contribute equally to vertical momentum flux, farther from the ground the flux is dominated by the low-speed regions. Furthermore, the pdfs of $u$ show that horizontal velocity is negatively skewed away from the ground indicating the predominance of low-speed streaks (Fig. 9).

6. Effect of subgrid-scale parameterization on ABL structure

We argued in section 3c that horizontal roll vortices observed in moderately convective boundary layers originate in near-ground low-speed streaks. A direct
consequence of this coupling between near-ground and mixed layer structure is that changes in SGS parameterization that alter near-ground structure can affect LES predictions of global ABL structure. We demonstrate this effect by comparing ABL structure predicted using the one-equation Smagorinsky-based SGS model implemented by Moeng (1984) with the more recent SGS parameterization by Sullivan et al. (1994).

The SGS parameterization implemented by Moeng overpredicts mean shear close to the ground (Sullivan et al. 1994; Khanna and Brasseur 1997). The modified Smagorinsky-based parameterization proposed by Sullivan et al. is designed primarily to reduce this over-prediction to values measured experimentally. Figure 31 compares the Monin-Obukhov-normalized mean shear profiles predicted by the two SGS closures for a moderately convective ABL state ($-\bar{z}/L = 8$). Because of the stronger mean shear, the near-ground streaky structure of the streamwise velocity fluctuations predicted by Moeng’s SGS scheme is more pronounced than that predicted by the Sullivan et al. SGS scheme. If the updrafts (forming the upward leg of the horizontal roll vortices) originate in these near-ground streaks as we have argued, their sheetlike structure should be significantly more coherent using the Moeng SGS scheme.

The effect of the SGS model on the near-ground struc-
ture of low-speed streaks is apparent in comparisons of isocontours of streamwise velocity using the Moeng parameterization in Fig. 32, with the contours of Fig. 18 using the Sullivan et al. model. Note that near the ground the predicted low-speed streaks are significantly more pronounced and elongated in the streamwise direction using the Moeng parameterization, a direct consequence of the higher local shear predicted with this parameterization.

Figure 33 shows a three-dimensional surface of high-intensity vertical velocity in the moderately convective ABL (–z_i/L = 8) simulated using SGS model employed by Moeng for comparison with the same ABL simulated in Fig. 15 using the Sullivan et al. SGS parameterization. The updrafts predicted using the Moeng parameterization (Fig. 33) are much more coherent than the updrafts predicted using the Sullivan et al. model. This obvious difference in streamwise coherence in vertical velocity predicted by the two SGS schemes is reflected quantitatively in Fig. 34 by a significantly larger ratio of streamwise to cross-stream integral length scale of vertical velocity using the Moeng SGS model.

We observe that, whereas the general features of horizontal rolls and sheetlike concentrations of vertical velocity are predicted using both the Moeng and Sullivan et al. parameterizations, the streamwise coherence of these structures is strongly affected by the parameterization. We argue that this difference in global structure of the atmospheric thermals is a direct consequence of the effects of the SGS parameterization on the local structure of the low-velocity streaks near the ground from which the atmospheric thermals arise (section 3c). This effect of the SGS model on the near-ground structure of low-speed streaks is apparent in comparisons of contours of streamwise velocity using the Moeng parameterization in Fig. 32, with the contours of Fig. 18 using the Sullivan et al. model. Near the ground the predicted low-speed streaks are significantly more pronounced and elongated in the streamwise direction using the Moeng parameterization. This increased elongation of low-speed streaks is a direct consequence of the higher local shear predicted using the Moeng parameterization.

7. Discussion

We have analyzed in some detail the local structure of primary energy-containing motions in the atmospheric boundary layer by combining classic statistical measures with 3D visualizations using large-eddy simulation data. By examining a wide range of –z_i/L states, we are able to discern the interaction of buoyancy and shear in the local and global structure of the ABL.

The convection-dominated boundary layer has been studied extensively in the literature. Our LES analysis
of local 3D structure of vertical velocity is consistent with previous observations where the buoyancy-induced updrafts form a turbulent Rayleigh–Benard cellular pattern with characteristic length scale of $z_i$ (Figs. 3–6). Close to the surface, small-scale thermal plumes emerge, grow with height, and merge with neighboring plumes to form large-scale, relatively uniform concentrations of upward-moving flow in the mid-boundary layer. This growth in the average scale of the vertical velocity eddies is reflected in a roughly linear increase in horizontal integral length scale of vertical velocity and a corresponding decrease in the wavenumber identifying the peak in the $w$ spectrum (Figs. 1–2). Our LES results are in close agreement with the field measure-
Fig. 28. Expected values of $w\theta$ conditioned on $w$ and normalized by the local mean at different $z/z_i$; $-\zeta/L = 8$. The dashed line (right-hand scale) is the pdf of $w$.

Fig. 29. Expected values of $uw$ conditioned on $w$ and normalized by the local mean $\bar{uw} < 0$ at different $z/z_i$; $-\zeta/L = 8$. The dashed line (right-hand scale) is the pdf of $w$. 

ments of integral length scales (Lenschow and Stankov 1986) and vertical velocity spectra (Kaimal et al. 1976).

Our simulations indicate a close resemblance between the structure of the neutral planetary boundary layer away from the capping inversion and the structure of other wall-boundary shear flows. Like the flat-plate boundary layer (FPBL), for example, the shear-induced structure close to the ground consists of alternating regions of low-speed and high-speed flow relative to the mean (Fig. 8). Also like the FPBL, the low-speed streaks are much more elongated in the streamwise direction than are the high-speed regions. However, we also observe a subset of low-speed streaks that extend through the boundary layer depth carrying momentum flux to the capping inversion and scaling on $z_i$ (Fig. 11). We argue that the subset of $z_i$-influenced low-speed streaks is enhanced by buoyancy forces at larger $-z_i/L$. At $-z_i/L = 0.44$, however, buoyancy forces are negligible, and near the surface the upward velocity fluctuations are concentrated in small-scale localized pockets along the low-speed streaks (Figs. 13–14).

In the moderately convective boundary layer, $z_i$-scale horizontal roll vortices aligned with the mean wind are observed in the simulated $-z_i/L = 3$ and 8 states (Fig. 17). Well-formed roll vortices have been analyzed by LeMone (1973) based on conditional averaging of the velocity field to determine the average “roll energy.” Our study adds a physically plausible argument for the mechanisms underlying the formation and organization of roll vortices.

We find that the coherent sheetlike updrafts, forming the upward legs of these horizontal roll vortices (Fig. 17),
15), originate close to the ground within the streamwise low-speed streaks. We argue that this origination of large-scale atmospheric thermals from near-ground streaks is a consequence of shear-induced dynamics that results in the concentration of upward-moving passive scalars within streaky regions of low-speed streamwise velocity fluctuations, commonly observed in measurements and simulations of wall-bounded shear flows with passive scalar. Whereas at small $-z/L$ temperature is a passive scalar with negligible buoyancy force, as $-z/L$ increases the concentration of warm fluid within the low-speed streaks gradually increases localized buoyancy forces and enhances the tendency for some low-speed streaks to extend to the capping inversion.

In contrast with the small-scale pockets of weak vertical motions along low-speed streaks in the neutral ABL (Fig. 13), in the moderately convective ABL the concentration of warm fluid within near-ground low-speed regions drives strong upward motions that merge in the streamwise direction near the ground, enhancing both vertical and streamwise coherence of the vertical velocity field (Fig. 15). We hypothesize that the downward motions that are created between these coherent sheets...
of vertical motion reduce or destroy the coherence of those near-ground low-speed streaks lying between the buoyancy-enhanced streaks (which scale on $z_i$). The net result, we argue, is the formation of large-scale streamwise aligned turbulent rolls that scale on $z_i$ but that are organized by shear-induced structure in the near-ground region of the surface layer.

Since the subgrid-scale (SGS) parameterization in large-eddy simulations has a significant impact on the local structure near the ground, the SGS parameterization should also affect global structure of the ABL. We show that because traditional Smagorinsky-based SGS schemes tend to overpredict mean shear in the surface layer of moderately convective boundary layers, this excessive shear enhances the streamwise coherence of near-ground streaks and therefore also the streamwise
coherence of the updrafts that originate from the near-
ground streaky structure (Figs. 31–34).

In the surface layer, there exists a disparity between the
characteristic length scales of the $u$ and $w$ fields.
The characteristic horizontal length scale of vertical ve-
clocity fluctuations scales with distance from the ground
in both shear and buoyancy-dominated boundary layers.
Because in buoyancy-dominated boundary layers streamwise velocity is strongly influenced by $z_i$, scale of
mixed layer eddies, $z_i$ is the characteristic length scale of
$u$ fluctuations. We find here that the near-ground streamwise velocity field in a shear-dominated boundary
layer ($-z_i/\lambda = 0.44$) also appears to be influenced by
$z_i$-scale outer eddies in that the characteristic length scales obtained from $u$ spectra (Fig. 10) and the average
streak spacing (Fig. 12) are of order $z_i$. This disparity has important implications in the boundary condition
for surface subgrid-scale momentum flux (Wyngaard
and Peltier 1996).

The structure of the temperature field is closely cor-
related with the local structure of the velocity field. In
moderately convective boundary layers, regions of high
temperature are correlated with regions of low-speed
streamwise velocity. The near-wall temperature field, there-
fore, has similar characteristic dimensions as low-
speed streaks. In a purely convective boundary layer,
the near-wall temperature field forms a cellular pattern
and regions of high local temperature near the ground
induce strong updrafts that grow in scale and intensity
from the ground to the mid boundary layer (Fig. 23).
Except near the capping inversion, these updrafts remain
correlated locally with high temperature (Figs. 4, 24).
Near the ground, however, the characteristic length scale of
temperature field in the surface layer is closer to the
characteristic length scale of the $u$ field than that of the
$w$ field (Fig. 1).

Based on sparse availability of spectral measurements
of temperature fluctuations within the surface layer, it
is generally assumed that under convective or moder-
ately convective conditions only the horizontal velocity fluctuations in this layer scale on $z$, (see Peltier et al.
1996). The current analysis of LES data, however, in-
dicates that temperature fluctuations within the surface
layer also scale on $z_i$. Moreover, we also observe this
outer scale influence in the near-neutral boundary layer.
Our analysis, therefore, suggests a stronger coupling
between the inner and outer regions of the boundary
layer than previously realized and calls for further in-
vestigation in this regard.

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Fig. 34. Effect of SGS parameterization on horizontal integral scales of $w$; $-z_i/\lambda = 8$. Solid line: using Sullivan et al. (1994) SGS model; dashed line: using the model in Moeng (1984).