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The effect of surface roughness on flow structures in a neutrally stratified planetary boundary layer flow

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The effects of surface roughness on the structures of a neutrally stratified planetary boundary layer flow are investigated by the large-eddy simulation technique. Our numerical model, which assumes horizontal periodicity, shows that the growth of an internal boundary layer (IBL) in response to an abrupt change of surface roughness (either smooth-to-rough transition or rough-to-smooth transition) obeys the 4/5th power of the time, similar to that along the downwind fetch. A sudden increase or decrease in the surface shear stress during the transition is also observed. A quadrant analysis shows that during the transition, ejections and sweeps are altered significantly. Flow visualization further illustrates that the distribution density and the strength of coherent vortical structures and ejection eddies increase substantially during the smooth-to-rough transition. Conversely, these parameters decrease in the rough-to-smooth transition. The mean velocity profile has an inflection point at the IBL top, but the coherent vortical motions and ejection eddies affected by the change of the roughness are inside the IBL, suggesting that this inflection point is more static than dynamic. We also compare the quasi-steady coherent flow structures of different surface roughness values after the transition period. Streak spacing appears to increase with increasing surface roughness. Ejection eddies and vortical structures increase in scale as well as in strength as the surface roughness increases. The correlation between drag coefficient and flow structures in boundary layer flows is discussed. © 1997 American Institute of Physics.

I. INTRODUCTION

Coherent structures within the planetary boundary layer (PBL) are of particular interest to PBL researchers because they have been found to dominate the turbulent transport of momentum, heat, and scalars (Wilczak and Tillman;1 Mahrt4). Recently, Lin et al.5 used a large-eddy simulation (LES) database to study the existence and role of coherent structures in a neutrally stratified PBL flow. Lin’s study identified coherent flux (low-speed ejections and high-speed sweeps) and vortical structures and emphasized the dynamic role of these structures in turbulence production and transport. Because of the varied, dynamic nature of the real-world atmospheric boundary layer, we should also investigate factors that may affect the scale and strength of these coherent structures. One of the conclusions from the work of Lin et al.5 is that in the shear-driven PBL, the surface layer serves as the origin for ejections and vortical events that in turn globally influence the properties of the PBL, suggesting that a change of the physical attributes of the surface layer may alter the scale and strength of these coherent structures. The present study focuses on the role surface roughness plays in the formation and evolution of coherent structures in a neutrally stratified PBL.

Many past studies have highlighted the role of surface roughness in fluid flow problems. For instance, it is well known that surface roughness increases friction drag (Schlichting) except for some particular surface geometric patterns, i.e.; riblets (Walsh), which can actually decrease friction drag compared to a smooth flat plate. Surface roughness also increases the vertical heat flux in convection flows (Shen et al.) by enhancing the emission of large thermal plumes from the boundary. In the convective PBL, Schmidt and Schumann7 also found that surface roughness affected heat transfer.

In the atmosphere, the PBL evolves over frequent abrupt changes of surface roughness, either from smooth to rough or from rough to smooth, leading to the formation of the IBL. The IBL is a reflection of the changing surface condition that develops within the existing PBL. Numerous past studies including those by Elliott,8 Panofsky and Townsend,9 Bradley,10 Peterson,11 Rao et al.,12 and Claussen,13 have advanced our understanding of the growth of the IBL and the structure of the PBL when advected over an abrupt change of surface roughness. One- or two-dimensional models developed by these researchers have reasonably predicted the growth of the IBL, the sudden increase or decrease of the surface shear stress, and the transitional wind profiles. But these studies did not report on changes in the three-dimensional coherent structures (e.g., ejections, sweeps, and

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vortices) during surface roughness transitions.

We speculated that a change in surface roughness could modify the coherent structures which in turn alter the global flow properties. In order to explore this issue, we examined the scale, intensity, and formation of coherent structures in a neutrally stratified PBL growing over three roughness heights. Furthermore, the transient phase of the PBL, when the roughness changes from either rough to smooth or smooth to rough is examined and compared to theories describing the growth of the IBL over inhomogeneous terrain.

The paper is organized in the following way. In section II, we present the numerical model and introduce the characteristics of the three different surface roughness cases used in the simulation. In section III, we discuss the effect of surface roughness on the mean velocity profiles. In section IV, we investigate the growth rate of the IBL after the surface roughness is changed from one case to another, and perform a quadrant analysis on the transitional flows to look into the changes in ejections and sweeps. Three-dimensional IBL flow structures are presented and discussed. In section V, we compare the quasi-steady flow structures, such as variances, streak spacing in the surface layer, and the outer-layer vortical structures among the three different roughness cases. We apply a three-dimensional conditional sampling technique to sample the ejection events to gain statistical information. In section VI, we discuss the implications of changing drag coefficient on flow structures. Concluding remarks are made in section VII. We also test the sensitivity of our results on the numerical grid mesh reported in the Appendix.

**II. NUMERICAL FORMULATION AND INITIAL CONFIGURATION**

The data were generated by a LES numerical code (Moeng; Moeng and Wyngaard), which solves time-dependent, incompressible Navier-Stokes equations with prescribed large-scale pressure-gradient and Coriolis forces. The effect of small turbulent eddies is parameterized through a subgrid scale (SGS) model developed by Sullivan et al. The lateral boundary condition is periodic, the bottom boundary matches the law of the wall at the first grid point above the surface, and the upper boundary allows upward radiation of internal gravity waves (Klemp and Durran). Initially, we impose an inversion layer at 2/3rd of the vertical domain where the temperature increases sharply with height. This capping inversion thus prevents the PBL from rapid growing. Below the capping inversion, the potential temperature tends to be well mixed after the turbulent motion is developed and thus remains rather uniform in height.

All three runs, NB, NR, and NS (see Table I), are driven by a geostrophic wind \((U_f, V_f) = (15, 0)\) m/s on a grid of 100×100×100 in a domain of 1500×1500×750 m³. The Coriolis parameter \(f = 10^{-4}\) s⁻¹. In all three cases, the PBL is neutrally stratified. NB, the baseline case, has a roughness height of 0.16 m. (N in NB stands for ‘neutral’ stratified PBL and B stands for ‘baseline’ case.) According to the table published by the Royal Aeronautical Society (Stull), this roughness height empirically corresponds to the terrain of “many trees, hedges, few buildings.” The rougher case, NR, has a roughness height of 0.83 m, corresponding to “center of large towns and cities;” the smoother case, NS, corresponds to “isolated trees, uncut grass,” with a roughness height of 0.018 m. All of the simulations were therefore conducted over land with fully rough surfaces. Note that over open water, the roughness height becomes quite small, e.g., \(z_0 \sim 10^{-4}\) m for flow over calm open seas (Stull).

The baseline case was first integrated for 53 large-eddy turnover times. Its flow properties were studied and presented in Lin et al. The PBL height, \(z_i\), is determined at the level where the mean potential temperature exceeds 0.25 of the layer-mean potential temperature, averaged from the bottom to this height; it is located right below the capping inversion. Cases NR and NS were initialized from the well-established turbulent flow of Case NB at 53 \(z_i/u_g\). Starting from this well-established turbulent flow, all three cases were run for approximately 10 additional large-eddy turnover times (which is about two hours of simulation). Data obtained during the first turnover time were used to study the transitional behavior due to a change in surface roughness. Then the flow returned to a quasi-steady state and the surface friction velocity remained approximately constant. Statistics were obtained from 20 3-D volumes sampled over the last five turnover times. Some flow properties of these three runs are given in Table I. We also performed a grid-refinement test (see Appendix) using a nested grid method (Sullivan et al.).

In this report, the spatial variables are \(x\), \(y\), and \(z\) and velocity variables are \(u\), \(v\), and \(w\), corresponding to the east, north, and vertical directions, respectively. Resolved variables (denoted by uppercase variables) are decomposed into horizontal means (uppercase variables with an overline) and fluctuating parts (lowercase variables); e.g., \(U = \bar{U} + u\). We use angle brackets \(\langle\rangle\) to indicate temporal averages.

**III. MEAN VELOCITY PROFILES**

The mean velocity profiles of the three runs are obtained by calculating horizontal and temporal averages over twenty instantaneous flow fields spanning the last five turnover times (about one hour of simulation time). Figure 1(a) shows that a rougher surface, which results in stronger surface shear

<table>
<thead>
<tr>
<th>Case</th>
<th>(z_0)</th>
<th>(z_i)</th>
<th>(u_g)</th>
<th>(\langle U_i(z_i) \rangle)</th>
<th>(z_i/u_g)</th>
<th>(u_g/U_g)</th>
<th>(c_f)</th>
</tr>
</thead>
<tbody>
<tr>
<td>NR</td>
<td>0.83</td>
<td>495</td>
<td>0.707</td>
<td>14.17</td>
<td>700</td>
<td>0.0471</td>
<td>0.00444</td>
</tr>
<tr>
<td>NB</td>
<td>0.16</td>
<td>459</td>
<td>0.633</td>
<td>15.15</td>
<td>710</td>
<td>0.0422</td>
<td>0.00356</td>
</tr>
<tr>
<td>NS</td>
<td>0.018</td>
<td>440</td>
<td>0.543</td>
<td>16.11</td>
<td>810</td>
<td>0.0362</td>
<td>0.00262</td>
</tr>
</tbody>
</table>

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stress or drag, slows down the mean speed \( \langle \bar{U}_s \rangle = \langle (U^2 + V^2)^{1/2} \rangle \) throughout the PBL, as expected. The mean momentum equations,

\[
\frac{\partial \bar{U}}{\partial t} + f(\bar{V} - V_g) - \frac{\partial \bar{w}}{\partial z} = -f(\bar{U} - U_g) - \frac{\partial \bar{w}}{\partial z},
\]

indicate that the change of mean velocity is primarily due to the vertical gradient of momentum flux caused by the surface roughness. If we normalize the mean speed by the speed at the PBL height [Fig. 1(b)], it becomes apparent that at the same dimensionless height, the vertical mean shear decreases with decreasing surface roughness except near the surface. That is, the same vertical mean shear as seen in the rougher case is found closer to the surface in the smoother case. This feature is similar to the increase of the free-stream velocity of smooth-wall flat-plate turbulent boundary layer (FBL) flows shown in Head and Bandyopadhyay\(^{20}\) and the change of smooth-wall to rough-wall in FBL flows shown in Krogstad et al.\(^{21}\) The PBL hodograph in Fig. 1(c) provides a sense of the wind veering; here the three arrows are the mean velocity vectors at the top of their respective PBLs. Near the surface the mean wind direction is approximately parallel to the mean shear direction and is about the same in the three runs. Even at the top of the PBL, the mean wind directions denoted by the arrows are about the same (only about one degree different). These computed mean speed profiles are also compared against the law of the wall; that is, \( \langle \bar{U}_s \rangle / u_\kappa = 1/\kappa \ln(z/z_0) \) where the von Karman constant, \( \kappa \), is 0.4, in Fig. 1(d). All three velocity profiles should collapse into a single line in the logarithmic region. Case NS appears to have a deeper surface layer in the \( z/z_0 \) coordinate because the value \( z_0 \) is smaller in this case. Qualitatively, decreasing

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure1.png}
\caption{(a) Mean speed \( \langle \bar{U}_s \rangle = \langle (U^2 + V^2)^{1/2} \rangle \) profiles; (b) normalized mean speed profiles \( \langle \bar{U}_s \rangle(z)/\langle \bar{U}_s \rangle(z_i) \) vs. \( z/z_i \); (c) wind hodograph; (d) normalized mean speed profiles \( \langle \bar{U}_s \rangle/u_\kappa \) vs. \( z/z_0 \); for Case NR, ---; Case NB, \( \cdots \cdots \); and Case NS, ----.}
\end{figure}
$z_0$ is analogous to an increase in Reynolds number (and a decrease in drag coefficient) in the smooth-wall FBL.

IV. FLOW STRUCTURES IN TRANSITION PERIOD

Cases NR and NS were initialized from the well-established turbulent flow of Case NB. Their flow fields before reaching a quasi-steady state thus represent the transition of flow structures from smooth-to-rough and rough-to-smooth conditions. During the transition, the IBL grows into the PBL top in about a large-eddy turnover time and the PBL thickness grows with the 4/5th power of the distance from the FBL origin. Because we change the surface roughness instantly and uniformly in space in our LES model, the growth of the IBL is with time, not with the fetch. In order to compare our flows with available IBL theories, we make the assumption that our homogeneous flow structures at any instant approximately correspond to inhomogeneous flow structures at a particular downwind fetch and that the relationship between time ($t$) and fetch ($x_f$) can be approximated by

$$x_f = C_v t,$$

where $C_v$ is a constant convective velocity. We have compared two IBL models with our LES results: the Elliott model (referred to as the E model) and the Panofsky-Townsend model (referred to as the P-T model). Although other more complicated two-dimensional models are available, such as Peterson and Rao et al., they are not substantially different from the simpler models.

The IBL depth given by the E model [equations (9) and (10) in Elliott] is

$$\eta = (0.75 - 0.03M) \xi^{0.8},$$

where $\eta = h/z_{02}$, $h$ is the IBL height; $M = \ln(z_{02}/z_{01})$; $\xi = x_f/z_{02}$; $z_{01}$ and $z_{02}$ are $z_0$ for $x_f < 0$ and $x_f > 0$, respectively. The depth $\eta$ varies as a 4/5th power of the downwind fetch. The P-T model [equation (8) in Panofsky and Townsend] has the following IBL depth-fetch relationship:

$$4k^2(\xi - \xi_0) = \eta \left[ \ln \eta - 5 + \frac{1}{2} M + \frac{4 - \frac{7}{2} M - \frac{1}{2} M^2}{\ln \eta - 1 + \frac{1}{2} M} \right. \right. \nonumber \left. \left. + \frac{4 + \frac{7}{2} M + \frac{1}{2} M^2 + \frac{1}{2} M^3}{(\ln \eta - 1 + \frac{1}{2} M)^2} \right] \right].$$

[Note that our definition of $M$ has an opposite sign to that of Panofsky and Townsend. In the P-T model, $\xi_0 = 0$ for $M = 1.65$ (smooth-to-rough transition) and $M = -2.17$ (rough-to-smooth transition). This relationship also yields a 4/5th power law. We define the IBL height, $h$, in the simulations as the height at which the mean wind speed is not influenced by the change of the surface condition; that is, the IBL height is the location where the difference between the mean speeds of the $z_{02}$ case and the $z_{01}$ case at the same

FIG. 2. Time histories of nondimensional surface shear stress: $z_{01} = 0.16m$, $z_{02} = (a) 0.83 m$ (smooth-to-rough transition); (b) 0.018 m (rough-to-smooth transition).
TABLE II. Average convective velocity, \( \langle C_v \rangle \) (m/s).

<table>
<thead>
<tr>
<th></th>
<th>( \langle C_v \rangle ) from E model</th>
<th>( \langle C_v \rangle ) from P-T model</th>
</tr>
</thead>
<tbody>
<tr>
<td>NB to NR (smooth to rough)</td>
<td>2.45</td>
<td>0.99</td>
</tr>
<tr>
<td>NB to NS (rough to smooth)</td>
<td>3.77</td>
<td>1.72</td>
</tr>
</tbody>
</table>

Simulation time is less than 1%. Using equation (2) in equations (3) or (4), we can estimate \( C_v \) from the simulations. This quantity was found to be approximately constant in time. This implies that the time evolution of the LES-simulated IBL also obeys the 4/5th power law.

The time-averaged \( C_v \) values (\( \langle C_v \rangle \)) are listed in Table II. Note that \( \langle C_v \rangle \) values estimated from the E model are more than two times larger than those from the P-T model (2.45/0.99 = 2.47 and 3.77/1.72 = 2.19). Panofsky and Townsend\(^9\) compared these two models and concluded that these two models agree very well except that at the same \( \xi \) (the downwind fetch normalized by the roughness height), the E model predicts a lower \( \eta \) (the IBL height normalized by the roughness height) than that of the P-T model. It is due to the difference in the definition of the IBL height. With our conditions, the ratio of the \( \eta \) obtained from the P-T model to the \( \eta \) from the E model at the same \( \xi \) varies from 1.6 to 5 and its average is about 2. Thus, in order to obtain the same \( \eta \) in the E model, the \( \xi \) and \( \langle C_v \rangle \) calculated from equations (3) and (2) should be about 2.37 times larger than those of the P-T model. Consistently, this value (2.37) is close to the above two ratios (2.47 and 2.19). Because the definition of the IBL height in this paper is similar to that of Panofsky and Townsend,\(^9\) the P-T model better represents our results. Since the convective speeds estimated from both models are close to the LES mean wind speeds near the surface shown in Fig. 1(a), it implies that the fetch-time relationship corresponds to the near-surface wind. Table II also shows that the convective velocity for the rough-to-smooth transition is higher than that of the smooth-to-rough transition, which is similar to the variation of mean speeds near the surface.

We then used the time-averaged \( C_v \) shown in Table II to construct the relationship between the corresponding fetch, \( \xi \), and the IBL height, \( \eta \), of the simulations shown in Fig. 3. The LES-simulated IBL height grows at a 4/5th power of the corresponding downwind fetch. The implication of the above analysis is that our LES flows during the transition from rough-to-smooth (or from smooth-to-rough) surface can represent the IBL flow structures at a corresponding downwind fetch.

C. Quadrant analysis

In both turbulent FBL and PBL flows, the ejections (low-speed negative momentum fluxes) are most active except very close to the surface, where sweeps (high-speed negative momentum fluxes) dominate. In this section, we investigate how each quadrant contribution of the momentum fluxes responds to the sudden change of surface roughness. We define a horizontal fluctuating velocity component, \( q \), shown below to simplify the presentation of the momentum fluxes \( u'w' \) and \( v'w' \) (Lin et al.\(^3\)):

\[
q = u \cos(\alpha) + v \sin(\alpha),
\]

where \( \alpha = \arctan(\nu'w''/\mu') \). The variable \( q \) is the horizontal fluctuating velocity component in the mean flux direction, which is approximately parallel to the mean shear direction in the surface layer. Superscripts + and − are used to indicate positive and negative fluctuating velocities. Thus, \( q^+ \) indicates a flux with \( q < 0 \) and \( w > 0 \), and hence denotes low-speed negative momentum fluxes; i.e., ejections. The quantity \( q^-w'' \) with \( (s,n) = (+,+),(-,+),(-,-),(+,-) \) represents the first, second, third, and fourth quadrants of the momentum fluxes, respectively. The second (ejection) and fourth (sweep) quadrant momentum fluxes contribute to positive production of turbulence. The first and third quadrant momentum fluxes contribute to negative production of turbulence.

We looked at the vertical distribution of the resolved momentum fluxes in the four quadrants about 202 seconds after changing the roughness height (not shown). It shows the dominance of ejection events away from the surface, with sweeps becoming more significant only very close to the surface. This general feature agrees with measurements of the turbulent flow above a pine forest (Bergström and Höögström\(^23\)) and in FBL flows (Robinson\(^23\)). In the smooth-to-rough transition, the vertical location of the maximum ejection strength is a little higher than that of sweep. The increase of ejection strength seems most significant for this scenario. To give a clearer picture of the quantitative difference in ejection and sweep behavior, we show the amount of increase of ejection and sweep strengths at two different time frames. Figure 4(a) shows the smooth-to-rough transition where (i) the maximum increase in ejection strength occurs at a higher altitude in the surface layer than that of sweep, and (ii) the ejection strength increases most significantly from 34% at \( t = 100 \) s and \( z/z_s \sim 0.08 \) to 50% at \( t = 202 \) s and \( z/z_s \sim 0.16 \). Similarly, Fig. 4(b) shows the rough-to-smooth transition, where ejection and sweep strengths decrease. This figure indicates that a sudden decrease of surface roughness
significantly weakens the ejection events in the whole surface layer and sweep events near the surface \((z \approx 0.1z_i)\).

A significant increase or decrease of ejection and sweep events suggests major changes in the activities of coherent motions, such as ejections, sweeps, collisions, and vortical structures during the transition, as will be demonstrated later.

**D. Coherent structures**

The three-dimensional coherent structures in a shear-driven PBL consist of ejection and sweep eddies and vortices. In the logarithmic region, the ejection eddies are elongated and vortices are smaller than those in the outer layer (Lin et al.\(^3\)). In this section, we investigate how ejections and vortical structures respond to the sudden change of surface roughness. We used the isosurface of the low-speed momentum fluxes \((q^-w^+)\) to identify ejections in the surface layer and the isosurface of the three-dimensional fluctuating pressure to define vortical structures during the transition period. The results (not shown) indicate that active flux and vortical structures become more sparse during the rough-to-smooth transition and vice versa, which is expected because the turbulence intensity weakens (or enhances) with a smoother (or rougher) surface. For low-Reynolds number, zero-pressure-gradient FBL flows, Robinson\(^{23}\) used quasi-streamwise and arch vortices to indicate vortices parallel and normal to the mean flow direction in the logarithmic region, respectively. Similarly, we found that the vortical structures in the transition period are either parallel or normal to the mean shear (or wind) direction in the surface layer. These vortices are strongly correlated with the flux structures (i.e., ejections). To give a clear picture of their relationship, we show a one-leg vortex parallel to the mean shear direction (a quasi-streamwise vortex) in Fig. 5, which appears during the smooth-to-rough transition. Its rotational feature is illustrated by the fluctuating velocity vectors [Fig. 5(d)] on a vertical plane normal to its front part [dashed line in Fig. 5(a)].
Sweeps (marked by B) and ejections (marked by C) are located on both sides of the vortex. Ejections are revealed by the surface-normal velocity vectors on the left-hand side of vortex A [around C in (d)]; that is, positive \( w \). We also examined the ejections and vortices in the undisturbed outer layer and found that they were almost identical for the three surface roughness cases.

In light of these observations, we conclude that the coherent flux and vortical structures within the IBL flows are similar to those found in the quasi-steady turbulent PBL flow. During the smooth-to-rough transition, stronger and more coherent flux and vortical structures are produced as the fetch increases. In the rough-to-smooth transition, the process is just the opposite. Since most of the ejections in the surface and outer layers originate near the surface \( \text{Lin et al.} \), the growth of the IBL may be attributed to the upward motions of ejections whose strength depends on the new surface roughness. These ejections are accompanied by vortices, as shown in Fig. 5.

### E. Inflectional mean speed profile

Previous field measurements and two-dimensional models of the IBL flows both exhibit an inflectional mean velocity profile at the interface of the IBL and an undisturbed outer layer flow \( \text{Petersen}^{11} \) and \( \text{Rao et al.}^{12} \). These features are also observed during the transition stage of our flows. Figure 6(a) shows the mean speed profiles at 202 seconds into the smooth-to-rough and rough-to-smooth transitions. The inflection points are obvious from the distribution of the vertical gradient of the mean speed \( \frac{d\overline{U}_s}{dz} \) shown in Fig. 6(b); that is, \( \frac{d\overline{U}_s}{dz} \) has a local maximum for the smooth-to-rough transition at \( z/z_i=0.2 \) and a local minimum for the rough-to-smooth transition at \( z/z_i=0.18 \), marked by A and B, respectively. The quadrant analysis and flow visualization of coherent ejection eddies suggest that the static inflection point may correspond to the height where the ejection eddies can reach at a particular time (or downwind fetch). For instance, inflection point A in Fig. 6(b) corresponds to the height where ejection strength has been affected in Fig. 6(c). Since these ejection eddies have strong negative fluctuating velocity component \( q \), they are very likely to modify mean velocity profiles and produce inflection points at the IBL top.

Further, the vertical distribution of the fluctuating vorticity \( \nabla \omega \) shown in Fig. 6(d) shows that vortical structures become more (or less) active in the whole IBL (not just at the inflection points) during smooth-to-rough (or rough-to-smooth) transition because vorticity magnitude in this region increases (or decreases). If an increase (or decrease) in strength of vortical structures indicates an increase (or decrease) in event of dynamic inflectional shear instability, the mean inflection point at the IBL top could fail to reveal the latter. Therefore, the inflection point at the IBL top may be more static than dynamic.

### V. DEPENDENCE OF FLOW STRUCTURES ON SURFACE ROUGHNESS

In this section, we investigate the nature of flow structures of the three roughness cases at quasi-steady state. First,
we look at the fluctuating velocity variance normalized by its own frictional velocity, $u_*^2$ [Fig. 7(a)], including the resolved and SGS parts. Note that $u_*^2$ increases with increasing $z_0$, as shown in Table I. Figure 7(a) shows that velocity variance scales well with $u_*^2$ throughout most of the shear-driven PBL except near the PBL top. Previous observed values of the normalized standard deviations of velocity fluctuations in the near-neutral surface layers of different sites indicate that $\sqrt{\langle uu \rangle}/u_* \approx 2.5$, $\sqrt{\langle vv \rangle}/u_* \approx 1.9$, $\sqrt{\langle wv \rangle}/u_* \approx 1.3$ (Stull\textsuperscript{18}). The peak standard deviation values in our surface layers are $\sqrt{\langle uu \rangle}/u_* \approx 2.1$, $\sqrt{\langle vv \rangle}/u_* \approx 1.7$, $\sqrt{\langle wv \rangle}/u_* \approx 1.2$. The agreement is quite good. Figure 7(b) shows that for $z/z_i \leq 0.5$, the value of $\sqrt{\langle pp \rangle}/\rho u_*^2$ is about the same regardless of the surface roughness. Note that fluctuating pressure is often used to indicate the strength of collisions and vortices. Given that turbulence is most active in the surface layer for a shear-driven PBL and that fluctuating pressure scales well with $u_*^2$ for $z/z_i \leq 0.5$, our simulations suggest that coherent vortical structures and ejection-related collisions increase in strength with increasing surface roughness. We also notice that data collapse near the PBL top is not good. It is probably because the important scales in the capping inversion are different from those in the bulk of the PBL due to the presence of entrainment and a stably stratified inversion. In the following subsections, we shall focus on the scale of the coherent structures within the PBL as a function of surface roughness height.

A. Low-speed streaks

Low-speed streaks are the fundamental flow structures in the surface layer (i.e., the logarithmic region) of shear-driven PBL flows, and they are strongly correlated with strong ejections in the PBL (Moeng and Sullivan\textsuperscript{24} and Lin et al.\textsuperscript{3}). Lin et al.\textsuperscript{3} showed that most ejections originate in the surface layer and spend their lifetime there. Some ejections in the outer layer evolve from the ejections in the surface layer (referred to as bursting process in FBL flows) and have a longer lifetime than those staying within the surface layer. The streaks are the source of turbulent motions in the PBL and play a significant role in turbulence production and dynamics.

A unique aspect of low-speed streaks in smooth-wall FBL flows is their spanwise spacing. Numerous investigations (e.g., Smith and Metzler\textsuperscript{25}) consistently show that the average streak spacing ($\bar{\lambda}^+$) for $z^+ \leq 5$ (where $z^+ = z u_*/v$, a wall unit) is invariant ($\bar{\lambda}^+ \approx 100$) over a wide range of Reynolds numbers. Values of $z^+$ less than or equal to 5 fall within the viscous sublayer, which does not exist in fully rough, high Reynolds number PBL flows. For $z^+ \geq 5$, $\bar{\lambda}^+$ was found to increase with increasing $z^+$. Nakagawa and Nezu\textsuperscript{26} compared $\bar{\lambda}^+$ at different values of $z^+$ from several independent measurements. Their results suggest that $\bar{\lambda}^+$ in the logarithmic region (i.e., our surface layer region) increases with increasing $z^+$; however, its value scatters and does not reach any constant value at the same $z^+$. When $z^+$ is further increased, $\bar{\lambda}^+$ gradually reaches an asymptotic relation of $\bar{\lambda}^+ \approx 2z^+$ in the outer layer. However, Smith and Metzler\textsuperscript{25} pointed out that streaks are a unique flow structure only near the surface and that they may not be clear and well defined in the outer layer. Thus, the above asymptotic relationship in the outer layer is questionable. Quantitative information on streak spacing in fully rough FBL flows is still lacking. The preliminary experimental results of FBL flows over rough walls by Grass et al.\textsuperscript{27} suggest that streak spacing should scale with roughness height.
In this section, we investigate the effect of surface roughness on the streak spacing of shear-driven PBL flows in the surface layer. Two-point correlation of the streamwise fluctuating velocity has previously been used successfully to estimate the average streak spacing (e.g., Kim et al.\textsuperscript{29}). In our flows, we compute the two-point correlation of the horizontal velocity component, $q$, defined by equation (5), which is the velocity component in the mean flux direction. The two-point correlation is given by

$$R_{qq}(r_1,r_2,z) = \frac{\langle q(x,y,z)q(x+r_1,y+r_2,z) \rangle}{\langle q^2(x,y,z) \rangle}.$$  

If the low-speed streaks are uniformly distributed and their spacing is about constant, the flow between low-speed streaks must be populated by high-speed streaks due to mass continuity. So, the distance between positive $R_{qq}$ at the origin and negative $R_{qq}$ represents the statistical distance between low-speed streaks and high-speed flow, and twice of this distance is the spatial and temporal average of streak spacing ($\bar{\lambda}$).

It is found that at the same height, $\bar{\lambda}$ increases with increasing surface roughness, $z_0$ (not shown). For the same $z_0$, the streak spacing increases linearly with height within the surface layer, in close agreement with field observations that show a linear increase with height of the spectral peak wavelength (Kaimal et al.\textsuperscript{29} and Lenschow\textsuperscript{30}). If we normalize $\bar{\lambda}$ and $z$ by $z_0$, as shown in Fig. 8(a), $\bar{\lambda}/z_0$ increases with decreasing $z_0$, for the same $z/z_0$. The dimensionless streak spacing in the logarithmic region is not constant and $\bar{\lambda}/z_0$ at different $z_0$ do not collapse into the same curve either, which are qualitatively consistent with results for the smooth-wall FBL flows (Figure 29 in Nakagawa and Nezu\textsuperscript{29}).

Instead of using the surface roughness for scaling, we scale $\bar{\lambda}$ and $z$ with the PBL height, $z_i$. Figure 8(b) shows that this scaling brings the three curves closer. Thus, we use linear regression method to fit these data to a straight line:

$$\frac{\bar{\lambda}}{z_i} = a + b \times \frac{\bar{\lambda}}{z_i},$$  

where $a = -0.24$, $b = 0.564$, $\sigma_a = 2.387 \times 10^{-2}$ and $\sigma_b = 3.383 \times 10^{-2}$. $\sigma_a$ and $\sigma_b$ are the standard deviations showing the probable uncertainties of parameters $a$ and $b$, respectively. This line is indicated by the “square” symbol in Fig. 8(b). Since $\sigma_a$ and $\sigma_b$ are less than 10% of their respective parameters, the line is a good fit.

Visual observation of low-speed streaks in our simulation data is straightforward. In Fig. 9, we show the contours of instantaneous strong negative $q$ at about 7.5 large-eddy turnover times into the transition. This figure illustrates plan views at $z/z_i=0.05$, 0.1, and 0.2 for the three cases. The $\bar{\lambda}$ values obtained from the two-point correlation are also indicated in these figures for comparison. These contour plots show that near the surface, the streaky feature is more pronounced and there are many fine-scale structures. With an increase in height, the streaks are disrupted and become wider, shorter and more intermittent, especially for the smaller surface roughness case. The wider streaks may be due to merging of thin streaks near the surface (Smith and Metzler\textsuperscript{25}) or the decrease of mean shear rate, which results in less stretched eddies. The shorter streaks at $z/z_i=0.2$, compared to those near the surface, also imply that all streaks have a hill and valley appearance. A plan view near the outer region of the surface layer merely cuts through the hills of the streaks, resulting in a shorter appearance of the streaks. Over a rougher surface [Figs. 9(a1), 9(a2), and 9(a3)], the large-scale streaks marked by $A$, $B$, and $C$ are stronger and quite persistent at different heights. Over a smoother surface, the large-scale streaks near the surface [Fig. 9(c1)] are not well defined at $z/z_i=0.2$ [Fig. 9(c3)]. These figures indicate that over a rougher surface, the streaks are bigger in the wall-normal ($z$) direction and that the smaller $\bar{\lambda}$ near the surface is due to the increase of fine structures. In the next section, we use a conditional technique to provide statistical information on structure size to support our visual observations.
B. Conditional sampling of ejection events

In this section, we investigate the size and strength of conditionally-sampled ejection eddies for different values of surface roughness height, and the magnitude of their associated vorticity. Although conditionally-sampled eddies do not necessarily correspond to an instantaneous flow structure, they represent the average flow structures around the detected events. The three-dimensional conditional sampling technique used by Lin et al. is adopted and is formulated as

\[
\hat{\Psi}(x', y', z') = \left( \Psi(x + x', y + y', z + z', t) \right)_{\text{cond}}, \tag{8}
\]

where \( \hat{\Psi}(x', y', z') \) is the conditional average of a physical quantity \( \Psi \), which is \( q^{-} w^{+} \) for ejection events and \( |\omega| \) for vortical events in which \( \omega \) is the fluctuating vorticity field, \( \% \) is the conditioning event, defined as \( q^{-} w^{+} u_{\text{w, NR}}^{2} < -1.25 \) for ejections at all \( (x, y, t) \) at a selected detection height, \( z \). This strict condition was used to detect and sample only strong ejection events. Two different detection heights were selected: \( z/z_i = 0.083 \) and \( 0.583 \).

Figures 10(a1), 10(b1), and 10(c1) show the top views of the isosurface of \( q w \) at \( z/z_i = 0.083 \) for Cases NR, NB, and NS, respectively. Figures 10(a2), 10(b2), and 10(c2) show
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Lin et al. 3 used the above conditional sampling technique to study a number of physical quantities, such as ejection events, pressure maximum and minimum, vorticity vectors (or vorticity line tracing), and vorticity magnitude. It is found that these conditionally sampled quantities correspond reasonably well to independent physical realizations of coherent motions in the turbulent flow. For example, the horseshoe-shaped $\overline{\omega}$ may represent the statistical average of the size and strength of vortical structures which satisfy the specified conditioning event. Therefore, we examined the conditional sampling of fluctuating vorticity magnitude, $\overline{\omega}$, associated with the above conditionally-sampled ejection events in the hope of providing some useful information about the size and strength of vortical structures as a function of surface roughness.

Figures 11(a1), 11(b1), and 11(c1) are top views of the conditionally-sampled ejections and the conditionally-sampled vortical events ($\overline{\epsilon}$) in the outer layer for the three roughness cases. Figures 11(a2), 11(b2), and 11(c2) are front views of these structures. Because $\overline{\omega}$ tends to incur a background vorticity sheet whose magnitude increases with decreasing height and because this sheet may connect to the trailing legs of a horseshoe-shaped $\overline{\omega}$ (Lin et al.), we chose an isosurface value for $\overline{\omega}$ such that the local maximum horseshoe-shaped $\overline{\omega}$ is separated from the background vorticity sheet (not shown), and the maximum is found to be located at the head of a horseshoe. The chosen isosurface value for $\overline{\omega}$ differs for the three cases: 0.0675, 0.062, 0.055 s$^{-1}$ for Cases NR, NB, and NS, respectively. We could have chosen the same isosurface value for the three cases, but we used different values for the following reason. If we apply $\overline{\omega} \geq 0.0675$ s$^{-1}$ to Cases NB and NS, the horseshoe-shaped isosurface disappears. Instead, the background vorticity sheet at a lower level than the detection height is captured. Apparently this threshold is too strict for these two cases. On the other hand, if we apply $\overline{\omega} \geq 0.055$ s$^{-1}$ to Cases NB and NR, the horseshoe-shaped isosurface is not adequately captured; instead a background vorticity sheet at a higher level is captured. These phenomena are caused by the fact that the strength of the background vorticity sheet not only increases with decreasing height at the same surface roughness but also increases with increasing surface roughness at the same height. By comparing Figs. 11(a1), 11(b1), and 11(c1) or 11(a2), 11(b2), and 11(c2), it appears that the horseshoe-shaped $\overline{\omega}$ maxima exhibit different scales at different levels of surface roughness. Although the NR case uses the strictest isosurface value, its sampled structure size is still the biggest, suggesting that statistically the vortical structures are stronger as well as bigger in PBL flows over a rougher surface. Also, Fig. 11 shows that the relative locations of flux (i.e., ejection) and vortical events are similar for different surface roughness heights.
Figure 12 shows the instantaneous vortical structures identified by strong negative fluctuating pressure, along with the streak-spacing distances at $z/z_i = 0.1$ obtained from the two-point correlation method. Two isosurface values are used; one uses the normalized fluctuating pressure value [Figs. 12(a), 12(b), and 12(c)], and the other uses the absolute fluctuating pressure value [Figs. 12(a), 12(b2), and 12(c2)]. Figures 12(a), 12(b), and 12(c) show that the vortical structures in all three cases are intermittent and that in each case they cover a wide spectrum of length scales. Nonetheless, larger horseshoe vortical structures are easier to be identified in the rougher surface case. Head and Bandyopadhyay have demonstrated that in smooth-wall FBL flows, the size of vortical structures (loops, horseshoes, and hairpins) in the outer layer approximately scales with the streak spacing in the viscous sublayer. This FBL finding appears to be consistent with what Figs. 12(a), 12(b), and 12(c) show. The difference in scales becomes more evident if we identify the vortical structures using the absolute pressure fluctuation, shown in Figs. 12(a), 12(b2), and 12(c2); there is a consistent reduction in the scale and strength of vortical structures as roughness height decreases. The variation of the strength of the vortical structures with the surface roughness is also consistent with the analysis of the standard deviation of fluctuating pressure in Fig. 7(b). Based on these data, we may conclude that in the neutrally stratified PBL, the scale and strength of vortical structures increase with increasing surface roughness.

VI. CORRELATION BETWEEN DRAG COEFFICIENT AND FLOW STRUCTURES

For smooth-wall FBL flows, Head and Bandyopadhyay have proposed that the parameter $U\delta/[v(c_f/2)^{1/2}]$ is of significance to coherent motions, where $U$ is the free-stream velocity, $\delta$ is the boundary layer thickness, $v$ is the kinematic viscosity, and $c_f$ is the drag coefficient $[=2(u^*/U)^2]$. This parameter depends only on the drag coefficient, $c_f$, because the Reynolds number $U\delta/v$, based on $\delta$, can be approximately expressed as a function of $c_f$ (Schlichting). Head and Bandyopadhyay have found that by increasing $U$, and hence the Reynolds number, the shape of vortical structures changes from loops to horseshoes, then to hairpins. That is, the vortical structures become narrower and smaller with decreasing drag coefficient (or $u^*/U$) since an increase of Reynolds number decreases $c_f$. Instead of increasing $U$, the same effect can be obtained by decreasing $u^*$, or the roughness height. Indeed, the foregoing results consistently show that by decreasing the surface roughness, and hence the drag coefficient, the size and strength of coherent ejections and vortices decrease. Recall that the mean speed at the PBL height [Table 1 and Fig. 1(a)] increases when $z_0$ decreases. Thus, decreasing $z_0$ can also indirectly create the effect of increasing the free-stream velocity. Our results reveal the correlation between drag coefficient and flow structures of shear-driven, boundary layer flows, and they suggest that altering the surface roughness has the same effect as altering the free-stream velocity or the Reynolds number.
VII. CONCLUSION

Using the LES technique, we were able to study the effect of surface roughness on flow structures in a neutrally stratified PBL flow. We focused on streak spacing, and the scale and strength of ejection eddies and vortical structures. We also investigated the transitional flow structures of the IBL when flows are changed from a smooth to rough surface or from a rough to smooth surface.

Our results indicate that the directions of the mean flow and shear in the surface layer remain approximately unchanged when the roughness height changes, but an increase in surface roughness slows down the mean speed throughout the whole PBL. In the smooth-to-rough or rough-to-smooth transition, the growth of the IBL appears to follow a 4/5th power law, as suggested by previous studies. Quadrant analysis indicates that during the transition, the strength of ejection and sweep events are both significantly affected. Flow visualizations and statistical analyses show consistently that a sudden increase of surface roughness increases the strength and the distribution density of both ejections and

![Figure 13: Two-point correlation $R_{qq}(r_1, r_2, z)$ of Case NS at (a) $z=22.5$ m, original non-nesting results; (b) $z=75$ m, original non-nesting results; (c) $z=22.5$ m, nesting results; (d) $z=75$ m, nesting results. $r_1$ and $r_2$ unit: meter.](image)
vortical structures. The movement of some of the ejections and vortical structures into the outer layer is responsible for the growth of the IBL.

A dimensionless parameter given by Head and Bandyopadhyay\textsuperscript{20} suggests that the drag coefficient (or the ratio of surface-friction velocity to free-stream velocity) is correlated to the scale and strength of coherent flux and vortical structures in the FBL flows. It has been demonstrated that streak spacing in the viscous sublayer of smooth-wall FBL flows (Smith and Metzler\textsuperscript{25}) and the size of vortical structures in the outer layer (Head and Bandyopadhyay\textsuperscript{20}) vary with the free-stream velocity, which leads to a change in drag coefficient and Reynolds number. In this study, we compared flow structures for different drag coefficients by varying the surface roughness, which effectively and directly changes the surface-friction velocity. It was found that the streak spacing in the surface layer appears to increase with increasing surface roughness, which is similar to an increase of drag coefficient in smooth-wall FBL flows.

Three-dimensional conditional ejection eddies in the surface layer are elongated in the mean shear direction. The strength and scale of these structures also increase with increasing surface roughness. The conditionally-sampled vortical eddies also increase in strength and scale with increasing surface roughness. Snapshots of instantaneous vortical structures of the three roughness cases show consistently that the vortical structures over a rougher surface are likely to be larger in scale. All of the above results indicate that the change of surface roughness in shear-driven PBL flows appears to have the same effect as the change of free-stream velocity in smooth-wall FBL flows. These results provide a possible explanation for the existence of large, strong horseshoe vortical structures in our shear-driven, fully rough PBL flow.

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APPENDIX: GRID-REFINEMENT TEST

A grid-refinement test was conducted to check our results of the small roughness case NS. Because a decrease in the roughness decreases the length scale of the coherent eddies, which are harder to resolve in LES, we performed the sensitivity test on grid resolution only for the smallest $z_0$ case. We adopted the nested grid method developed by Sullivan \textit{et al.}\textsuperscript{19} for the current LES model. In this grid nesting scheme, the grid architecture consists of a single outer (or coarse) grid and (single or multiple) overlapped, nested (or fine) grids. For our configuration, we nested a fine grid with grid points of $200 \times 200 \times 30$ in a physical domain of $1500 \times 1500 \times 22.5$ m$^3$ near the surface onto the original coarse grid ($100 \times 100 \times 100$) which covers the whole simulation domain ($1500 \times 1500 \times 750$ m$^3$). As a result, the vertical grid resolution within the fine mesh domain is 0.75 m. The communication between the fine and coarse grids is accomplished by a pressure matching method that implicitly matches the total flux on the grids in the overlap region. This type of matching is equivalent to using Germano’s identity (Germano \textit{et al.}\textsuperscript{31}) which is frequently used for dynamic SGS models. We carried out this simulation and generated quasi-steady data, about two large-eddy turnover times (the required computational time for 10 large-eddy turnover time was excessive more than 1000 Cray hours). Since the streak lifetime is about half of one large-eddy turnover time (Lin

FIG. 14. Low-speed streaks (contours of $q < -1$ m/s) for Case NS from the nesting run at (a) $z = 22.5$ m (from the coarse grid); (b) $z = 21.75$ m (from the fine grid). Darker regions correspond to a stronger negative $q$. Length unit: meter.
et al.) and our primary objective is to examine the sensitivity of the streak spacing to grid resolution, the statistics from the nested run based on the average of 20 3-D volumes spanning two large-eddy turnover times was considered adequate.

Figure 13 shows two-point correlations $R_{qq}$ at $z = 22.5$ m [i.e., $z/z_i = 0.05$, the same height as that shown in Fig. 9(c1)] and 75 m obtained from the original and nested runs of Case NS. It indicates that the average streak spacing $\langle \lambda \rangle$ from both runs is about the same at the same height. Furthermore, Fig. 14 shows contours of the instantaneous low-speed streaks obtained from the fine grid at $z = 21.75$ m and coarse grid at $z = 22.5$ m at the same time. (For the present nested grid architecture it is not possible to have data at precisely the same height in the overlap region, see Sullivan et al.) The figure shows that the elongated energy-containing eddies resolved by the coarse grid [Fig. 14(a)] are almost identical to those obtained from the fine grid although the latter reveals more detailed subgrid structures. We also examined the percentage of resolved and subgrid-scale (SGS) flux as a function of height. With the nested grid, the fraction of resolved flux increases from 72% to 88% at the 3rd vertical grid point of the coarse grid ($z = 3$, $z/z_i = 22.5$ m, and $z/z_i = 0.05$). Above this level (i.e., $z/z_i = 0.05$), the percentage of unresolved SGS flux drops to less than 10% very quickly, indicating that most of energy-containing eddies are resolved. Therefore, we concluded that the flow structures in the original Case NS with $z/z_i = 0.05$ are adequately resolved.