The role of coherent structures in subfilter-scale dissipation of turbulence measured in the atmospheric surface layer

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Abstract. A field experiment was designed and carried out to study the role of coherent structures on the local transfers of energy and temperature variance between resolved and subfilter (unresolved) scales relevant to large-eddy simulation of high-Reynolds-number boundary layers. In particular, 16 sonic anemometers were used in an arrangement with a 6 m high vertical array (ten anemometers) that intersected a 3 m wide horizontal array (seven anemometers). The data collected are used to calculate the subfilter-scale (SFS) stresses and fluxes, and the SFS dissipation rate (transfer rate between resolved and subfilter scales) of energy and temperature variance. With these quantities, conditional averaging is used to study the relation of strong positive (forward-scatter) and negative (backscatter) SFS dissipation events to local features of the flow. The conditionally averaged vertical and horizontal flow fields reveal vortical structures, inclined downwind at angles close to 16° during near-neutral atmospheric stability, and as large as 34° during convective conditions. These inclined vortical structures agree with the concept of a hairpin vortex (with head and trailing legs) around which sweep and ejection events are found. Localized regions of large forward-scatter are found on the upper trailing edge of these structures, whereas localized regions of large backscatter are found on the lower leading edge of the same type of structures.

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1. Introduction

Accurately simulating turbulent transport in the atmospheric boundary layer (ABL) across a wide range of spatial and temporal scales is of key importance to understand better land–atmosphere interactions for a variety of conditions. To this end, large-eddy simulation (LES) has become a popular tool to study the influence of atmospheric stability and heterogeneous surface conditions on the fluxes of momentum, heat, water vapour and pollutants in the ABL (e.g. [1]–[13]). LES provides the unique ability to simulate three-dimensional (3D), unsteady transport of momentum and scalars (e.g. temperature, moisture, pollutants) resolved down to scales of the order of a few metres. To do this, the LES method uses spatial filtering to remove small, unresolved (spatial and temporal) scales and parametrizes their effect on the resolved scales using a subfilter-scale (SFS) model.

The success of LES relies on the ability of the SFS models to reproduce the effects of the unresolved (subfilter) scales on the resolved scales accurately. Improving these models has been identified as the foremost challenge to address in order to make LES a more applicable and reliable tool to study high-Reynolds-number flows [14]–[16]. Two general approaches have been used to improve SFS modelling: (a) a posteriori studies that analyse turbulent fields from simulations with different SFS models and (b) a priori studies that analyse high-resolution turbulence data obtained from direct numerical simulations or direct measurements of turbulence. While a posteriori studies are the ultimate tests of SFS models, the bias due to the numerical methods and the choice of SFS model limit the understanding that can be gained from the results. Specifically, results from a posteriori studies cannot provide any information about the interactions between the resolved and subfilter scales, since they are parametrized by the SFS model used in the simulation. A priori studies, on the other hand, provide information both on the subfilter and resolved scales and allow for the study of the relation between the two which is essential to make fundamental improvements in SFS model formulations.

Originally, a priori studies for LES were performed in low-to-moderate Reynolds number flows using high-resolution turbulence data from laboratory (wind tunnel) measurements (see e.g. [17]–[20]) and also from direct numerical simulations (see e.g. [21]–[24]). More recently,
a series of \textit{a priori} studies has been carried out in the high-Reynolds-number ABL (e.g. [25]–[31]). These studies have provided useful information about the essential properties of SFS physics and on the performance of current SFS models.

An open issue in SFS modelling within LES is related to the lack of understanding of the connection between SFS parametrizations and the local dynamics of the flow. Specifically, intermittent transfers of energy and temperature (scalar) variance between resolved and subfilter scales have been problematic to modelling. This includes the transfer of energy or scalar variance from unresolved scales to resolved scales, also known as backscatter, which is counter to the mean forward cascading process of turbulence. Typical SFS models such as the eddy-viscosity (or eddy-diffusivity) model fail to produce backscatter. Works by Porté-Agel \textit{et al} [25]–[28] used field measurements and \textit{a priori} testing of SFS eddy-diffusion models to show this failure. Porté-Agel \textit{et al} [27, 28] also used conditional averaging to associate strong intermittent transfers of scalar variance between resolved and subfilter scales with temperature ramp-structures associated with sweep and ejection events. Lin [32], using results from an LES of a convective ABL, associated both positive and negative ‘near-grid-scale’ transfers of energy with sweep and ejection events, also using conditional averaging. The results presented by Lin [32] include the effect of an SFS eddy-viscosity model and thus do not provide information on the behaviour of the SFS physics. Other studies in the ABL have associated non-Gaussian behaviour of turbulent measurements with sweep and ejection events [33]–[36]. In fact, significant percentages (75% and more reported by Gao \textit{et al} [37] and 90% by Högström and Bergström [34]) of turbulent fluxes have been attributed to sweep and ejection events, believed to occur around coherent structures. Although it is often agreed that turbulent fluxes and energy transfers between resolved and subfilter scales are due to local flow phenomena [32], no clear evidence exists, to date, of the specific role that 3D coherent structures play in SFS transfers in LES.

A substantial amount of experimental and numerical studies have determined various types of coherent structures commonly found in turbulent boundary layers (see the review by Robinson [38]). An inclined vortical structure emanating from the lower surface with a horseshoe shape, first suggested by Theodorsen [39], has become a well accepted model for the fundamental structure found in the logarithmic velocity region of turbulent boundary layers. Conditional averaging and two-point correlations have been widely used in the past to determine the average characteristics of these structures [40]–[42]. Brown and Thomas [42], using two-point correlations, determined that the inclination angle of these structures is approximately 18°. Similar to the horseshoe-shape vortex, hairpin-shaped vortices were observed by Head and Bandyopadhyay [43] and were shown to travel in groups. These hairpin vortices are characterized by a core vorticity surrounded by sweep and ejection events and a local increase of shear stress and scalar flux. Recent experiments in the atmospheric surface layer by Hommema and Adrian [44] visualized local inclined structures that support the hairpin-vortex-packet theory developed by Adrian \textit{et al} [45]. This theory coupled with a kinematic model based on Townsend’s attached eddy hypothesis [46, 47] has been shown by Marusic [48] to agree with measured statistics of high-Reynolds-number boundary layers. A recent study by McNaughton [49] has also recognized the importance of Townsend’s attached eddy hypothesis by determining that turbulent spectra calculated from experimental data measured in the ABL are consistent with the concept of wedge-like coherent structures as the primary contributors to active turbulence in a neutrally buoyant surface layer.

This paper reports results from an \textit{a priori} field study with a similar experimental setup to those of Porté-Ágel \textit{et al} [26]–[28], using arrays of sonic anemometers. In contrast to those studies, this study uses 16 sonic anemometers in an arrangement with a 6 m high vertical array (ten anemometers) that intersected a 3 m wide horizontal array (seven anemometers) and has a central goal of providing information about the association of SFS dissipation of energy and
scalar variance with 3D coherent structures. In the following section we present the equations solved by LES, define the SFS quantities important to modelling and describe the type of measurements required to evaluate such quantities. In section 3, we describe the experimental setup, the resulting high-resolution turbulence data and how we used these data to calculate SFS fluxes and transfer rates of energy and scalar variance. In section 4, we present results of our study that highlight the structure of the flow using conditional averaging techniques along with two-point correlations of the velocity and temperature data. Section 4 also discusses a proposed conceptual model that relates important SFS dynamics with local flow features. Conclusions on this work are given in section 5.

2. LES

In LES, resolved flow variables (components of velocity and scalars) are defined by a spatial filtering operation at a scale $\Delta$:

$$\tilde{\alpha}(x) = \int \alpha(x') G_\Delta(x - x') \, dx',$$

(1)

where $\alpha$ is a flow variable, tilde denotes the filtered quantity and $G_\Delta$ is the 3D filter function. The scale $\Delta$ (of the order of 10 m in the ABL) determines the spatial resolution of the simulation and is at least equal to, if not larger than, the computational grid size $\Delta_{LES}$. Applying the filter kernel, $G_\Delta$, to the equations governing the conservation of mass, momentum and scalars in the ABL, yields the equations solved by LES:

$$\frac{\partial \tilde{u}_i}{\partial x_i} = 0,$$

(2)

$$\frac{\partial \tilde{u}_i}{\partial t} + \frac{\partial \tilde{u}_i \tilde{u}_j}{\partial x_j} = -\delta_{ij} \tilde{T}_v = \langle \tilde{T}_v \rangle - \frac{\rho}{\rho} \frac{\partial \tilde{p}}{\partial x_i} - \frac{\partial \tau_{ij}}{\partial x_j},$$

(3)

$$\frac{\partial \tilde{\theta}}{\partial t} + \frac{\partial \tilde{u}_i \tilde{\theta}}{\partial x_j} = -\frac{\partial q_i}{\partial x_i},$$

(4)

where $\tilde{u}_i$ (using index notation) represents the three components of filtered velocity, $\tilde{T}_v$ is the filtered potential virtual temperature, the brackets $\langle \rangle$ are used to represent a horizontal average, $\tilde{T}_0$ is a reference temperature, $f_c$ is an angular velocity that accounts for Coriolis effects, $\rho$ is the density of air, $\tilde{p}$ is the filtered pressure and $\tilde{\theta}$ is a scalar quantity (e.g. temperature, water vapour or pollutant concentration). Buoyancy effects in the conservation of momentum equation are accounted for by using the Boussinesq approximation [1]. The terms $\tau_{ij}$ and $q_i$ are the SFS stress tensor and SFS heat flux, respectively, and are defined as

$$\tau_{ij} = \tilde{u}_i \tilde{u}_j - \tilde{u}_i \tilde{u}_j,$$

(5)

$$q_i = \tilde{u}_i \tilde{\theta} - \tilde{u}_i \tilde{\theta}.$$

(6)

These SFS stresses and fluxes are unknown quantities and must be modelled within LES. Modelling of these SFS stresses/fluxes, while important throughout the ABL, becomes critical in the surface layer where the flow is more anisotropic due to the increased shear near the surface. Many traditional SFS models rely on the assumption that scales exhibiting local isotropy (inertial-subrange scaling) are partially resolved. However, in the surface layer, the filter scale is of the order of (or even larger than) these locally isotropic scales. Due to this scaling range
limitation, subfilter scales near the surface have a larger contribution to the overall turbulent flux, and thus are more challenging to model [14, 16].

The effects of $\tau_{ij}$ and $q_i$ on the resolved flow variables can be examined by considering the evolution equations for the resolved kinetic energy, $K = \frac{1}{2}\tilde{u}_i\tilde{u}_i$, and the resolved scalar variance, $\mathcal{K} = \frac{1}{2}\tilde{\theta}^2$, respectively. The evolution equation for the resolved kinetic energy [21] is

$$\frac{\partial K}{\partial t} + \tilde{u}_j \frac{\partial K}{\partial x_j} = -\tilde{u}_3 \frac{\tilde{T}_v - \langle \tilde{T}_v \rangle}{\tilde{T}_\theta} g + f_c \epsilon_{ij3} \tilde{u}_i \tilde{u}_j - \frac{1}{\rho} \frac{\partial \tilde{u}_i}{\partial x_i} \left( \frac{\partial \tilde{u}_i}{\partial x_j} - \Pi \right) - \chi.$$  \hspace{1cm} (7)

The last term in this equation is the SFS dissipation rate of energy, $\Pi = -\tau_{ij} \tilde{S}_{ij}$, where $\tilde{S}_{ij} = \frac{1}{2}(\partial \tilde{u}_i/\partial x_j + \partial \tilde{u}_j/\partial x_i)$ is the filtered strain rate tensor, and represents the transfer of kinetic energy between resolved and subfilter scales. The evolution equation of filtered scalar variance [25] is

$$\frac{\partial \mathcal{K}}{\partial t} + \tilde{u}_j \frac{\partial \mathcal{K}}{\partial x_j} = -\frac{\partial q_i \tilde{\theta}}{\partial x_i} - \chi.$$  \hspace{1cm} (8)

This equation includes a scalar SFS dissipation (or transfer) term, $\chi = -q_i(\partial \tilde{\theta}/\partial x_i)$, that represents the transfer of scalar variance between resolved and subfilter scales. The SFS dissipation rates, $\Pi$ and $\chi$, have special importance since accurately reproducing their mean values has been found to be a necessary condition for LES to yield correct flow statistics [14].

On an average, the values of $\Pi$ and $\chi$ are positive, indicating net transfers of energy and scalar variance, respectively, from larger scales to smaller scales. However, the time histories of $\chi$, based on the field measurements, reveal highly intermittent positive and negative values [27, 28]. Negative values of these SFS dissipation rates indicate a transfer of energy or scalar variance from small (subfilter) scales to large (resolved) scales, or backscatter. Probability density functions (PDFs) of $\Pi$ and $\chi$, also taken from field measurements, suggest that these backscatter events occur over a range of values and contribute significantly to the overall transfers of energy and scalar variance across the filter scale [27, 30]. The localized intermittency of $\Pi$ and $\chi$ is representative of the complex, non-linear physical interactions occurring across the filter scale. This behaviour of $\chi$ has been linked in recent a priori studies to temperature ramps along with sweep and ejection events in the atmospheric surface layer using conditional averaging of temperature and velocity measurements [27, 28]. Furthermore, traditional eddy-diffusion (Smagorinsky) SFS models have been found, by the same field studies, to fail in reproducing these interactions. Eddy-diffusion models and for that matter eddy-viscosity models are fully dissipative by design and, therefore, unable to produce backscatter (transfer of scalar variance or energy from subfilter scales to resolved scales).

Providing improved SFS models that accurately account for the effect of coherent structures on the localized SFS transfers of energy and scalar variance is essential to improve the accuracy of LES of the ABL. Identifying the role of coherent structures requires new experimental designs that can characterize, simultaneously, SFS transfers and 3D flow structures. In this paper, we present results from a field study using arrays of sonic anemometers in the atmospheric surface layer. High-resolution measurements of velocity and temperature are used to compute SFS stresses and heat fluxes as well as SFS dissipation rates of energy and scalar variance at one location in the surface layer. At the same time, our measurements also provide information about the flow structure (characterized using temperature and velocity fields) surrounding that location. Results from this study can be used in a posteriori studies to test the ability of different LES–SFS schemes to capture the local transfers of energy and scalar variance, and their relation with coherent structures. These results can also provide guidance for the development of new SFS models. The next section describes the details of the field study and the data acquired.
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Figure 1. Sketch of (a) front view and (b) top view of the measurement array. The heights of the sensors are indicated in (a) and the required shift of the data-sets (to align the axes with the mean wind) as well as the shift’s effect on the horizontal spacing of the anemometers are depicted in (b). The shaded circle represents the position at which SFS dissipation rates were estimated.

3. Experimental setup

3.1. Experimental setup and measurements

The field experiment took place at the Surface Layer Turbulence and Environmental Science Test (SLTEST) facility located on the salt flats in the Great Salt Lake Desert of Western Utah during July 2002. The site consists of a flat, dry lake-bed that has a homogeneous fetch of at least 50 km in prevailing wind directions. The landscape surrounding the SLTEST site can be best described as having sparse desert vegetation with cracks formed at the surface. The aerodynamic roughness height, $z_0$, is estimated from velocity profiles to be approximately 0.5 mm.

The experimental setup involves 16 tri-axial sonic anemometers (Campbell Scientific CSAT3s) measuring the three components of velocity and temperature. The sonic anemometers are arranged forming a setup with a vertical array (up to 6 m) and a horizontal array, intersecting each other at the midpoint of the horizontal array located at a height of 1.9 m as depicted in figure 1. The data were collected by data-loggers (Campbell Scientific CR5000’s) sampling at a frequency of 20 Hz. Time series were logged continuously through various atmospheric stability conditions over an entire diurnal cycle (14:00, 24 July to 14:30, 25 July). The original data were separated into 30-min periods and individual subsets were selected based on the level of stationarity of wind direction, wind speed and turbulent statistics. Data-sets obtained during periods in which the mean wind approached the arrays at an angle ($\beta$ in figure 1) greater than 35° were not considered to avoid flow distortion due to the tower supporting the sensors.
Table 1. Mean wind and atmospheric conditions calculated based on 5-min averages for data taken on 24–25 July 2002 at the SLTEST facility.

<table>
<thead>
<tr>
<th>Time series</th>
<th>Local time</th>
<th>$\bar{u}_1$ (m s$^{-1}$)</th>
<th>$\beta$ (°)</th>
<th>$\bar{\theta}$ (K)</th>
<th>$u_*$ (m s$^{-1}$)</th>
<th>$z/L$</th>
<th>$\sigma_{u_1}$ (m s$^{-1}$)</th>
<th>$\sigma_{\theta}$ (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>D1</td>
<td>17:05–17:35</td>
<td>7.7</td>
<td>−32.9</td>
<td>308.8</td>
<td>0.31</td>
<td>−0.18</td>
<td>0.88</td>
<td>0.46</td>
</tr>
<tr>
<td>D2</td>
<td>17:55–18:25</td>
<td>12.3</td>
<td>0.8</td>
<td>306.5</td>
<td>0.45</td>
<td>−0.11</td>
<td>1.48</td>
<td>0.25</td>
</tr>
<tr>
<td>D3</td>
<td>18:45–19:15</td>
<td>7.3</td>
<td>−30.3</td>
<td>305.6</td>
<td>0.29</td>
<td>−0.06</td>
<td>1.08</td>
<td>0.17</td>
</tr>
<tr>
<td>N1</td>
<td>00:45–01:15</td>
<td>6.4</td>
<td>11.1</td>
<td>295.1</td>
<td>0.22</td>
<td>0.02</td>
<td>0.76</td>
<td>0.06</td>
</tr>
<tr>
<td>N2</td>
<td>02:55–03:25</td>
<td>4.1</td>
<td>10.6</td>
<td>294.6</td>
<td>0.13</td>
<td>0.10</td>
<td>0.33</td>
<td>0.07</td>
</tr>
<tr>
<td>N3</td>
<td>04:05–04:35</td>
<td>3.2</td>
<td>−5.7</td>
<td>294.3</td>
<td>0.13</td>
<td>0.02</td>
<td>0.34</td>
<td>0.05</td>
</tr>
<tr>
<td>D4</td>
<td>08:35–09:05</td>
<td>5.0</td>
<td>−7.9</td>
<td>296.1</td>
<td>0.20</td>
<td>−0.24</td>
<td>0.49</td>
<td>0.25</td>
</tr>
<tr>
<td>D5</td>
<td>09:05–09:35</td>
<td>4.1</td>
<td>−19.2</td>
<td>296.5</td>
<td>0.16</td>
<td>−0.81</td>
<td>0.38</td>
<td>0.31</td>
</tr>
<tr>
<td>D6</td>
<td>09:35–10:05</td>
<td>4.0</td>
<td>−13.9</td>
<td>297.3</td>
<td>0.11</td>
<td>−3.12</td>
<td>0.53</td>
<td>0.38</td>
</tr>
<tr>
<td>D7</td>
<td>11:55–12:25</td>
<td>3.4</td>
<td>−11.7</td>
<td>300.4</td>
<td>0.17</td>
<td>−2.39</td>
<td>0.96</td>
<td>0.74</td>
</tr>
</tbody>
</table>

Atmospheric stability during each measurement period was characterized by the Obukhov length,

$$L = \frac{-u_*^3(\theta)}{\kappa g \langle u_*'^3 \theta'^3 \rangle},$$

where $u_*$ is the friction velocity, $\kappa$ the von Kármán constant (taken here to be 0.4), $g$ the gravitational acceleration and the prime (') denotes fluctuation from a time average (represented here by brackets). Table 1 shows mean wind and atmospheric conditions along with the local time for each data-set. To calculate the statistics for each time period (as presented in table 1), non-stationary trends in the time series were removed using averages based on 5 min increments of the data as suggested by Vickers and Mahrt [50]. Other methods were also evaluated, such as a wavelet-based detrending algorithm and a high-order polynomial fit, but the results did not change significantly.

The mean wind direction, $\beta$ (see figure 1), is calculated based on the mean values of the horizontal components of velocity. This direction is used to align the time series with the mean wind such that $X$ is the streamwise direction, $Y$ the spanwise direction and $Z$ the vertical direction. To account for the true spanwise direction, the time series across the horizontal array are shifted, with the midpoint of the array as the pivot point using Taylor’s frozen-flow hypothesis. This is done so that the time series are virtually parallel to one another and synchronized. The resulting shift is small due to the limited range of $\beta$, and has little effect on the results. The spacing between the sensors in the horizontal array is 0.5 m before adjustment by the shift. A photograph of this experimental setup at the SLTEST site is shown in figure 2.

Taylor’s hypothesis is often used in the analysis presented here. The use of Taylor’s hypothesis has been well accepted for data measured in the atmospheric surface layer with turbulence intensities up to 30% and more [51]. The turbulent intensities calculated from the data included in this study are generally around 10% and all are less than 30%. Further discussion of the use of Taylor’s hypothesis and feasibility of using sensor arrays to study SFS quantities in the atmospheric surface layer can be found in Tong et al [29].

3.2. Data quality and experimental error

The power spectra calculated from the three components of velocity measured at a height $z = 1.9$ m for one of the time periods selected are shown in figure 3. The spectra are normalized
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Figure 2. Photograph of the field study setup at the SLTEST facility on the salt flats in Western Utah. The setup consists of 16 sonic anemometers positioned along vertical and horizontal arrays, crossing at 1.9 m above the desert floor.

Figure 3. Normalized power spectra of the three components of velocity (---, streamwise-velocity spectrum; ····, spanwise-velocity spectrum; ---, vertical-velocity spectrum) corresponding to data-set D4. The characteristic $-5/3$ slope in the inertial subrange and $-1$ slope in the production range are also indicated. The vertical arrow points out the scale at which the filtering operation is applied (see section 3.3).

using the friction velocity ($u_*$) and the height at which the measurement was taken ($z$). The normalized spectra show an inertial subrange (with approximate $-5/3$ slope signifying locally isotropic turbulence) across normalized wavenumbers ranging from the height of the
Role of coherent structures in SFS dissipation measurement, $k_1 z = 1$ (where $k_1$ is the streamwise wavenumber and is calculated using Taylor’s hypothesis), to the resolution limit of the sensor. Spectra obtained from the other data sets are similar to those shown in figure 3 and exhibit a wide dynamic range of measurements. The filter scale is shown in the figure (arrow pointing to normalized wavenumber $(\pi/\Delta) z$) to fall in the mid-section of the inertial subrange.

A source of error when calculating SFS stresses and fluxes comes from the limitation in measurement resolution as a result of the path length (10 cm) and sampling frequency (20 Hz) of the sonic anemometers. This limitation, however, is of little consequence to our results here since we are filtering at scales that are an order of magnitude larger $(\Delta = 2.0 \text{ m})$. Previous studies have found that the dominant contribution to SFS stresses/fluxes comes from scales that are in the vicinity of $\Delta$, mostly from the neighbouring octave and not from scales that are much smaller [14, 27, 52].

Manufacturer specifications of accuracy for the sonic anemometers used with digital communication to the data-loggers are 0.2–2 mm s$^{-1}$ for velocity and 0.002°C for temperature fluctuations. This error corresponds to at most 0.6% of the standard deviation for velocity and 4% of the standard deviation for temperature. For each sensor there is also a possibility of bias errors that can shift the mean values of the signals without affecting the fluctuations. The impact of these bias errors is small, however, since they have no effect on SFS stresses/fluxes, and the contribution of the mean gradients to the mean SFS dissipation rates is only of the order of 5%. Errors due to flow distortion caused by the presence of the supporting towers or other sensors is thought to be negligible. The towers were designed to have minimal cross-sectional profile and the velocity spectra (figure 3) suggest no corruption by flow distortion at high wavenumbers.

3.3. Subfilter-scale quantities

SFS stresses ($\tau_{ij}$, equation (5)) and fluxes ($q_i$, equation (6)) were computed using a 1D streamwise filter with a width of $\Delta = 2.0 \text{ m}$ in the streamwise direction (applying Taylor’s hypothesis). Higher-order (2D and 3D) filtering is not possible due to the limited spatial coverage of the sensors. The effects of the filter dimension and the use of Taylor’s hypothesis in the streamwise direction have been reported to affect the calculated SFS quantities only in their magnitude, but not in their relative significance and behaviour [26, 29]. Thus, the qualitative conclusions of this study are not expected to be affected by the filter dimension and the use of Taylor’s hypothesis. The streamwise filtering operation was performed using three different filter types common in LES: the Gaussian, top-hat (sharp cut-off in wavenumber space) and box (sharp cut-off in physical space) filter functions [15]. After evaluating our results using each of these filter functions, we found that our conclusions were not significantly changed by the choice of filter. Consequently, here we only present results obtained with a Gaussian-filter function. This function has a smooth behaviour and is defined in wave space as $\hat{G}_\Delta(k_1) = \exp[-k_1^2\Delta^2/24]$, where $k_1$ is the wavenumber. The filtering operation was applied by convolving in wave space the Fourier transform of the measured data with the Gaussian-filter function defined here.

The gradients of the filtered velocity and temperature were computed along all three axial directions at the location where the vertical and horizontal arrays intersect. This was done using a centred finite-differencing scheme with the filtered data from the nearest sensors for the spanwise and vertical gradients, and the filtered data from the time series at half the filter scale (invoking Taylor’s hypothesis) for the streamwise gradients. This information was then used to compute the SFS dissipation rates as defined in section 2. Representative samples of the time series of the SFS scalar dissipation rate $\chi$ and SFS energy dissipation rate $\Pi$ are shown in figure 4. They both exhibit large intermittency and numerous occurrences of
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Figure 4. Sample time series of (a) SFS dissipation rate of scalar variance $\chi$ and (b) SFS dissipation rate of resolved energy $\Pi$ for data-set D1.

Table 2. Mean and standard deviation values for the SFS dissipation rate of scalar variance ($\chi$) and energy ($\Pi$) corresponding to different measurement periods.

<table>
<thead>
<tr>
<th>Time series</th>
<th>Start time</th>
<th>$\langle \chi \rangle \times 10^4$ (K$^2$s$^{-1}$)</th>
<th>$\sigma_{\chi} \times 10^3$ (K$^2$s$^{-1}$)</th>
<th>$\langle \Pi \rangle \times 10^3$ (m$^2$s$^{-3}$)</th>
<th>$\sigma_{\Pi} \times 10^2$ (m$^2$s$^{-3}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>D1</td>
<td>17:05</td>
<td>28.0</td>
<td>35.2</td>
<td>7.13</td>
<td>18.02</td>
</tr>
<tr>
<td>D2</td>
<td>17:55</td>
<td>7.22</td>
<td>15.40</td>
<td>31.0</td>
<td>77.2</td>
</tr>
<tr>
<td>D3</td>
<td>18:45</td>
<td>3.87</td>
<td>6.20</td>
<td>7.63</td>
<td>19.99</td>
</tr>
<tr>
<td>N1</td>
<td>00:45</td>
<td>0.227</td>
<td>0.456</td>
<td>3.24</td>
<td>8.50</td>
</tr>
<tr>
<td>N2</td>
<td>02:55</td>
<td>0.168</td>
<td>0.191</td>
<td>0.597</td>
<td>2.00</td>
</tr>
<tr>
<td>N3</td>
<td>04:05</td>
<td>0.366</td>
<td>2.75</td>
<td>0.001</td>
<td>5.04</td>
</tr>
<tr>
<td>D4</td>
<td>08:35</td>
<td>5.60</td>
<td>7.10</td>
<td>1.009</td>
<td>3.30</td>
</tr>
<tr>
<td>D5</td>
<td>09:05</td>
<td>8.82</td>
<td>10.18</td>
<td>0.508</td>
<td>2.08</td>
</tr>
<tr>
<td>D6</td>
<td>09:35</td>
<td>15.10</td>
<td>12.23</td>
<td>4.30</td>
<td>3.72</td>
</tr>
<tr>
<td>D7</td>
<td>11:55</td>
<td>54.9</td>
<td>76.0</td>
<td>0.872</td>
<td>6.35</td>
</tr>
</tbody>
</table>

backscatter (negative values). The statistics of the SFS quantities calculated from the data-sets are summarized in table 2.

As mentioned in section 2, traditional eddy-viscosity and eddy-diffusion models used in LES do not account for backscatter (or transfer of energy from subfilter scales to resolved scales) of scalar variance or energy. However, the SFS quantities calculated from the measurements made directly in the atmospheric surface layer reveal significant negative occurrences of $\chi$ and $\Pi$. Here, we analyse the PDFs of the SFS fluxes and dissipation rates from a typical data-set (D1). The
Figure 5. Probability density functions of the components of SFS scalar fluxes $q_i$ for data-set D1. The thick solid line represents the Gaussian distribution.

Figure 6. Probability density functions of the components of SFS stresses $\tau_{ij}$ for data-set D1. The thick solid line represents the Gaussian distribution.

plots in figure 5 show PDFs of the three components of the SFS heat flux $q_i$. These PDFs show non-Gaussian behaviour identified by the raised, non-zero PDF tails. PDFs of the components of SFS stresses $\tau_{ij}$ are shown in figure 6. These PDFs also show a non-Gaussian behaviour, with asymmetric PDF tails. These results agree well with other similar measurements in the ABL by Porté-Agel et al [26]–[28] and Higgins et al [30]. The PDFs of SFS dissipation rates of scalar variance and energy (both shown in figure 7) have significant occurrences of negative values.
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Figure 7. Probability density functions of the SFS dissipation rate of scalar variance $\chi$ and SFS dissipation rate of resolved energy $\Pi$ for data-set D1. The thick solid line represents the Gaussian distribution.

(backscatter). The mean values of $\chi$ and $\Pi$ (see table 2) generally decrease with increasing atmospheric stability as a consequence of the overall damping of turbulence associated with flow stratification.

Porté-Agel et al [25]–[28] have related sweep and ejection events with positive and negative SFS dissipation rates of scalar variance in the ABL and studied the effect of filter scale and atmospheric stability on SFS physics. However, the 3D structure and vortical nature (used to define coherent structures) of the flow surrounding non-Gaussian, intermittent SFS dissipation are yet to be determined. The next section uses conditional averaging techniques to deduce the nature of the local flow structure associated with significant occurrences of positive and negative SFS transfers of energy and scalar variance.

4. Results and discussion

4.1. Conditional averaging and coherent structures

The local flow conditions that contribute to significant positive and negative SFS dissipation rates are studied by conditionally sampling flow properties (temperature, velocity and vorticity) based on strong (positive or negative) events of $\chi$ and $\Pi$. The events are selected from the time series based upon excursions of SFS dissipation rates beyond thresholds that are proportional to mean values of the SFS dissipation rates. 2D windows (from the horizontal and vertical arrays) of data (temperature, velocity and vorticity) surrounding locations where these extreme events occur are sampled and averaged together. The windows are converted from temporal to spatial
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Figure 8. Vertical fields of conditionally averaged temperature fluctuations $\theta'(K)$ with overlaid conditionally averaged fluctuating velocity vectors for positive and negative SFS dissipation rates of energy under weakly unstable conditions (data-set D1). Flow is from left to right and every other vector in the streamwise direction has been removed for visual purposes.

Dimensions using Taylor’s hypothesis. This conditional averaging procedure is defined as

$$
\langle \Phi \mid C \rangle(x', y, z) = \frac{1}{N} \sum_{n=1}^{N} \Phi(x_n + x', y, z),
$$

where $\Phi$ is the flow quantity sampled (e.g. temperature, velocity or vorticity), $x_n$ (with $1 \leq n \leq N$) are the points where the condition $C$ is satisfied, $N$ is the number of events satisfying this condition and $X$ is the length of the conditionally sampled window. The condition $C$ is defined (for example, based on $\Pi$) as either $\Pi(y=0.0\ m, z=1.9\ m) > 5\langle \Pi \rangle$ for forward-scatter events or $\Pi(y=0.0\ m, z=1.9\ m) < -3\langle \Pi \rangle$ for backscatter events. The levels of the thresholds ($5\langle \Pi \rangle$ and $-3\langle \Pi \rangle$) have been chosen to be large enough to isolate the local effects, but small enough to guarantee convergence to the mean flow away from the location of the SFS dissipation event. The same threshold coefficients (+5 and −3) are applied to obtain conditional averages based on $\chi$.

The vertical field of conditionally averaged temperature based on strong-positive SFS dissipation rates (forward-scatter) of energy and scalar variance is presented in figures 8(a)
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Figure 9. Vertical fields of conditionally averaged temperature fluctuations, \( \theta' (K) \), with overlaid conditionally averaged fluctuating velocity vectors for positive and negative SFS dissipation rates of scalar variance under weakly unstable conditions (data-set D1). Flow is from left to right and every other vector in the streamwise direction has been removed for visual purposes.

and 9(a), respectively. Positive SFS dissipation events (at the location marked with a ‘+’ in figures 8(a) and 9(a)) tend to occur at the interfaces of relatively warmer air (from below) and cooler air (from above). The fluctuating-velocity-vector field (also conditionally averaged) shows that near the forward-scatter events there is typically a convergence of the flow with the inception of an ejection (velocity directed upwind and away from the surface) below the event location. For strong-negative SFS dissipation rates (backscatter, see figures 8(b) and 9(b)), the events tend to take place at divergences in the flow with a volume of warm air being ejected away from the event location. Note that the results of the conditional averages based on either the SFS dissipation rate of energy (II, figure 8) or the SFS dissipation rate of scalar variance (\( \chi \), figure 9) support the same conclusions regarding the local flow properties around strong-positive and strong-negative SFS dissipation events. Seemingly, figures 8(a) and (b) and figures 9(a) and (b) suggest that different regions surrounding an ejection of relatively warmer air appear to be associated with completely opposite signs of SFS dissipation.

Next, the conditional averaging procedure is applied to the vorticity fields to obtain a clearer picture of the ‘average flow structure’ associated with strong forward and backward scatter events. The vertical field of conditionally averaged vorticity (spanwise component only)
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Figure 10. Vertical fields of conditionally averaged spanwise vorticity $\omega_y$ (Hz) for positive and negative SFS dissipation rates of energy under weakly unstable conditions (data-set D1). The ‘+’ indicates the location at which the SFS dissipation rates satisfy the threshold condition.

corresponding to the strong-positive SFS dissipation rates (figures 10(a) and 11(a)) shows a region of vorticity which is inclined downwind (at approximately 15–20°) with a core of vorticity located downwind and above the SFS dissipation events. The conditionally averaged flow field surrounding the backscatter events (figures 10(b) and 11(b)) also has a core region of positive vorticity; however, in this case it is located upwind and above the SFS dissipation events. Results from figures 8–11 indicate that the conditionally averaged vertical fields of temperature, velocity and vorticity, associated with strong positive and negative SFS transfers, are qualitatively the same for both energy and scalar variance. The same conclusions are found for other conditionally averaged fields considered and, therefore, only results corresponding to SFS energy dissipation are presented next.

To understand better the three-dimensionality of the flow structures surrounding these SFS dissipation events, horizontal fields of conditionally averaged temperature and vorticity (vertical component only) were calculated corresponding to the same SFS dissipation events used to conditionally average vertical fields. The horizontal fields of conditionally averaged temperature are presented in figure 12. These results show that strong forward-scatter and backscatter occur respectively, downwind (figure 12(a)) and upwind (figure 12(b)) of regions of relatively warmer air. These warm air regions are the same that appear in the vertical fields shown in figures 8 and 9, and they are associated with ejection events that carry relatively warmer air upwards. The
Figure 11. Vertical fields of conditionally averaged spanwise vorticity $\omega_y$ (Hz) for positive and negative SFS dissipation rates of scalar variance under weakly unstable conditions (data-set D1). The ‘+’ indicates the location at which the SFS dissipation rates satisfy the threshold condition.

The horizontal field of conditionally averaged vorticity (figure 13(a)) for the forward-scatter events shows two pairs of counter-rotating vortices on either side of the centre-spanwise line on which the SFS dissipation events occur (at $x' = 0\, \text{m}$, $y = 0\, \text{m}$). Note that the dominant pair of vortices is downwind of the forward-scatter events. Around the backscatter events (figure 13(b)), the dominant vortex pair is shifted with respect to the pair in the forward-scatter events and is located upwind of the backscatter event.

The conditionally averaged plots presented here (figures 8–13) are based on thousands of realizations of the turbulent flow and are highly indicative of a fundamental coherent structure characterized by the outline of the vorticity contours. For a more detailed understanding and explanation of these contour patterns, we consider previous experimental studies of coherent structures in lower (moderate) Reynolds-number boundary layers [39, 41, 43, 45]. Conceptual models from these experimental results suggest that coherent structures in the logarithmic layer have hairpin-like structures with characteristic inclined legs with opposite rotations, extending upward and meeting to form a core of spanwise vorticity at a head. Our results agree with these conceptual models as one can trace out the silhouette of hairpin vortices in our conditionally averaged fields (both vertical and horizontal). The rotation of the core of the vortices in the horizontal field agrees with two downward extending legs that have opposite signs of vorticity and directly contribute to the ejection events shown in the velocity field of figures 8 and 9. Based on
Figure 12. Horizontal fields of conditionally averaged temperature fluctuations, \( \theta'(K) \) for positive and negative SFS dissipation rates of energy under weakly unstable conditions (data-set D1). Flow is from bottom to top. The ‘+’ indicates the location at which the SFS dissipation rates satisfy the threshold condition.

Figure 13. Horizontal fields of conditionally averaged vertical vorticity \( \omega_z \) (Hz) for positive and negative SFS dissipation rates of energy under weakly unstable conditions (data-set D1). Flow is from bottom to top. The ‘+’ indicates the location at which the SFS dissipation rates satisfy the threshold condition.
our results, a conceptual model is proposed (figure 14) that positions strong positive SFS dissipation (again forward-scatter) events on the upper trailing edge of hairpin-like structures and the negative SFS dissipation events (backscatter) on the lower leading edge of the same hairpin-like structures. Although the occurrence of forward-scatter and backscatter may in reality be more intricately attached to these structures, we limit our interpretation to what we observe in our conditionally averaged results. Conditionally averaged vertical fields (not presented here) based on a 2D surrogate SFS dissipation rate calculated at varying heights along the vertical array show that the height (scale) of the structure in this model is found to be directly proportional to the height at which the SFS dissipation rate is computed and conditionally sampled. A 2D surrogate of the SFS dissipation rate is calculated along the vertical array since spanwise gradients cannot be computed. This conclusion agrees with Townsend’s attached eddy hypothesis [46] and the kinematic model of Perry et al [47] which assume that the logarithmic layer of a turbulent boundary layer is populated with coherent structures of different scales that vary with distance from the surface.

4.2. Two-point correlations and atmospheric stability effects

In order to obtain quantitative information about the inclination of coherent structures in the atmospheric surface layer, two-point correlations have been calculated between the streamwise-velocity time series at different vertical positions. Once the correlations were calculated, the lag in the streamwise direction was converted to space scales using Taylor’s hypothesis and a
constant convection velocity. The correlation function is then defined as

$$R(r) = \frac{\langle u_{(1)}(x)u_{(\ell)}(x + r) \rangle}{\sigma_{u_{(1)}}\sigma_{u_{(\ell)}}},$$

(11)

where $r$ is the spatial streamwise separation at which the correlation is computed, $u_{(1)}$ is the streamwise-velocity time series from the lowest anemometer, $u_{(\ell)}$ is the streamwise-velocity time series from measurements along the vertical array of anemometers with $\ell = 2$–10, representing the measurement positions along the array (index increasing with height) and $\sigma_{u(-)}$ is the standard deviation of the velocity time series. We assume that the value of the convection velocity is equal to a local mean velocity. Although the correlation function is calculated over the entire data-set and not just the portions associated with localized events of SFS dissipation, the contributions of the inclined structures are evident in the lag to maximum correlation found at different heights. Figure 15(a) shows the result of the two-point correlations of streamwise velocities. By finding the lag of the maximum correlation between each pair, a linear relation can be found (by least-squares fit) between the measurement height and the lag associated with the maximum correlation. The arctangent of the slope yields a characteristic inclination angle along which the maximum correlations occur. One such measurement of lag to maximum correlation (for data-set D4) is shown in figure 15(b). The angles determined from these maximum correlations are shown versus atmospheric stability in figure 16. For near-neutral conditions, our results suggest that the atmospheric surface layer has structures with a characteristic inclination angle of about 16°. This is in good agreement with the angles found from previous laboratory experiments [42, 45]. Our results also suggest that the effect of positive buoyancy during highly unstable conditions ($z/L < -1$) produces a substantial increase in the characteristic inclination angle of the flow structures, reaching values as large as 34° (see figure 16).
Figure 16. Angle of inclination found from lags at maximum correlation between velocity time series measured at different heights (see figure 15), plotted as a function of the atmospheric stability parameter, $z/L$ (measured at a height of 4.9 m).

Figure 17. Conditionally averaged vorticity fields for two different time periods: (a) near-neutral conditions (from data-set N2) and (b) unstable conditions (from data-set D7). The ‘+’ indicates the location at which the SFS dissipation rates satisfy the threshold condition. The dashed lines correspond to the inclination along the angles determined from the two-point correlation analysis.
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This effect of atmospheric stability on the inclination of the conditionally averaged structures presented in figures 8–13 is further illustrated in figure 17 in which conditionally averaged fields from two data-sets with different atmospheric stability are considered. Figure 17 shows vertical fields of conditionally averaged vorticity for data-set N2 with $z/L = +0.10$ (weakly stable conditions, top panel) and data-set D7 with $z/L = -2.39$ (unstable conditions, bottom panel). From visual inspection, the angle of inclination of the conditionally averaged vorticity contours matches well with the values obtained from the peak correlations (shown as dashed lines in figure 17). The increase in the inclination angle of flow structures associated with positive buoyancy (unstable atmospheric conditions) as previously shown in figure 16 is also evident from the conditionally averaged structures in figure 17.

5. Summary and conclusions

A field experiment was designed and carried out to study the role of coherent structures on the local transfer of energy and temperature variance between resolved and subfilter scales relevant to LES of high-Reynolds-number boundary layers. In particular, 16 tri-axial sonic anemometers were used in an arrangement with a 6 m high vertical array (10 anemometers) that intersected a 3 m wide horizontal array (seven anemometers). The data collected were used to compute the SFS stresses and fluxes using a Gaussian filter applied in the streamwise direction employing Taylor’s hypothesis. Furthermore, the filtered strain rate and gradients of the filtered temperature are computed at the crossing-point of the two arrays, and used to calculate the SFS dissipation rate (transfer between resolved and subfilter scales) of energy and temperature variance. Conditional averaging is used to study how strong positive (forward-scatter) and negative (backscatter) SFS transfer rates are related to the local flow structure as measured with the two arrays.

Horizontal and vertical fields of conditionally averaged velocity, vorticity and temperature based on strong positive and negative SFS dissipation of energy and scalar variance show that forward-scatter and backscatter are associated with different locations around hairpin-like vortex structures. These structures are similar to those reported in previous studies of low and moderate Reynolds number boundary layers. A conditionally averaged hairpin-like structure is identified by an intense vortex core in the vertical plane and by two counter-rotating vortices, corresponding to the two downward extending legs, in the horizontal plane. The rotation of this coherent vortex contributes to (if not produces) the ejection event seen in the conditionally averaged velocity and temperature field. Strong forward-scatter of energy and scalar variance is found to occur on the upper-trailing edge of the hairpin vortex at a convergence in flow above an ejection event. Conversely, strong backscatter of energy and scalar variance is found to be associated with the lower leading edge of the same type of hairpin vortex, where a divergence of the flow occurs at the lower edge of an ejection event. A 3D conceptual model of the flow surrounding these strong SFS dissipation events is presented that illustrates the findings from the conditionally averaged fields.

The characteristic angles of structures in the flow were quantified using two-point correlations calculated between the streamwise velocity time series along the vertical array. These angles varied between $15^\circ$ and $35^\circ$ and were found to be a function of atmospheric stability. Under near-neutral conditions, the characteristic inclination angle is about $16^\circ$, which is in good agreement with previous studies in moderate-Reynolds-number flows. Under convective (unstable) conditions, positive buoyancy forces the characteristic angle of the structures to be larger than during neutral and slightly stable conditions.

In the context of LES, we present unique experimental evidence from the atmospheric surface layer for the qualitative role of coherent structures (using 3D information) on the
local intermittent nature of the transfers (forward-scatter and backscatter) of energy and scalar variance between resolved and subfilter scales. This information is suitable to be used in a posteriori studies to evaluate the performance of current and newly developed SFS models based on their ability to capture the local structure and dynamics of the flow. These efforts also complement analytical and conceptual models of the fundamental structures of turbulent boundary layers which may lend guidance to the development of improved SFS parametrizations.

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