Response to reviewers

Turbulence vertical structure of the boundary layer during the afternoon transition

We thank the reviewers for their helpful and constructive comments, which helped us to improve the manuscript.

All of the specific comments have been taken into account.

In response to the reviews we have modified some parts of the manuscript, including:

- An improved discussion concerning the different TKE decay regimes found in our study compared with literature,
- An improved discussion concerning the 'top-down' decay of turbulence found in LES.
- A more exhaustive bibliography connected with our findings,
- Complementary information on the LES model and the numerical settings (subgrid model, boundary conditions...),
- Missing acronyms definition
- Revisiting the spectra shape and scales changes based on a better analysis of Figure 8,
- Rewriting of the sentences which were not clear to the reviewers,
- Changing Figure 4: the new Figure 4 shows less profiles, with different colors used for more clarity, as suggested by reviewer 1.
- Adding the initial LES profiles of $\theta$ and wind direction on Figure 2.

Below there is a copy of the reviewer 1 comments (in italic and blue), with a detailed response to each point.

Responses to Reviewer 1:

GENERAL COMMENTS:
The paper deals with an interesting problem of the boundary layer meteorology. The turbulence decay at the sunset is reproduced and analyzed using a LES model coupled with experimental data that are acquired during the BLLAST field experiment. This experiment is an international cooperation between some European Institutions and NCAR. The results show some interesting and new aspects that merit to be published. Besides that, I have the following two questions.

- The first main conclusions drawn from this study is that the decay process is generically divided in two phases, which is the early afternoon (0-0.75 $\tau_f$) and late afternoon (0.75 $\tau_f$ - 1.0 $\tau_f$). In which way this is compatible with the recent findings in which the exponent of the decay rate has instead three different scaling regimes ($t^{-1}$, $t^{-2}$, $t^{-6}$) ?????

Our finding is that the TKE decay follows two main stages: we define the first period that we call the early afternoon in the temporal range from 0 to 0.75 $\tau_f$ and then the late afternoon (from 0.75 $\tau_f$ to 1.0 $\tau_f$). This result remains consistent with the recent findings of three stages in Rizza et al. (2013a), based on LES. The difference comes from the way of defining those stages. Figure 1 represents the temporal evolution of the coefficient -n which governs the TKE decay following a power law in $t^n$ when representing TKE/$w_*^2$ as a function of $t/t_*$ with a log-log representation. The expression reads:

$$\log\left(\frac{TKE}{w_*^2}\right) = -n \log\left(\frac{t}{t_*}\right).$$
This coefficient evolves all along the afternoon period (see Fig. 1). Since the coefficient tends progressively from 0, to very large negative values of \(-n\), we find actually somehow arbitrary to define a specific value for this coefficient that would characterize the different phases of the TKE decay. For example, Nadeau et al. (2011) defined two stages defined by the power laws \(t^{-2}\) and \(t^{-6}\) (see Figure 3 (b)) whereas Rizza et al. (2013a) added a preliminary phase in \(t^{-1}\) (see Figure 2 (a)). Our first stage includes \(t^{-1}\) and \(t^{-2}\) power laws, and the second one includes \(t^{-6}\). Note that the goal of our study is rather to link the decay stages with the evolution of the turbulence structure.

We have rewritten the manuscript to connect our findings in relationship with the recent findings in section 5.4, lines 807:

“The two stages of the TKE decay found in this study remain consistent with previous results found by Nadeau et al. (2011) and Rizza et al. (2013a). Both authors showed a decrease of the TKE following a \(t^{-n}\) power law with a continuous increase of \(n\). Nadeau et al. (2011) defined two main stages characterized by \(n\) around 2 and 6 respectively. Rizza et al. (2013a) added a preliminary stage with \(n\) equal to 1. Our first stage includes \(t^{-1}\) and \(t^{-2}\) power laws, and the second one includes \(t^{-6}\). However, it seems somehow arbitrary to characterize our two stages by a specific value of \(n\) since it evolves continuously. This study focuses on the link between the structure of the turbulence and the TKE evolution.”

Figure 1: Temporal evolution of the coefficient \(n\) which governs the TKE decay following a power law in \(t\) when representing \(\text{TKE}/w^2\) as a function of \(t/t_\tau\) with a log-log representation with LES data. Time is normalized so that the afternoon transition starts at 0 and ends at 1.
The second important point concerns the “turbulent evolution along the vertical”. An important conclusion is that the decay occurs first at the top of the boundary-layer then it propagates downward toward the surface. But as the authors declared, there are some “noticeable differences” (pag.32503, line 15) between the observed and simulated mean profiles (fig.4) and for the TKE (fig.7) as well. Furthermore, the estimation of $z_i$ underestimates the observations while the surface stability conditions are not discussed at all. So, I think that these aspects should be more deeply investigated and in particular if this conclusion is not influenced by the poor LES prediction of mean and turbulent quantities.

As the reviewer correctly mentioned, there are some noticeable differences between the LES and the observations. But our aim was not to reproduce a real case. We have modified the text in Section 3, l.263 to clarify this point:

“As a complementary tool, a LES is initialized with the BLLAST observations to study turbulence decay over an homogeneous and flat surface. The observations of the 20 June are used to guide our simulation, like the 1 July and 25 June guided the studies of Blay et al. (2014) and Pietersen et al. (2015) respectively. Our aim is not to reproduce a real case but rather to use the BLLAST dataset as a benchmark to simulate a boundary layer with the same range of thermal and dynamical instabilities than those observed during BLLAST.”

The difference in terms of stability and wind shear are discussed in the response to the specific comments.

Moreover, despite the simulation shows a 'top-down' decay of turbulence, we are not sure that it actually occurred in the reality for this day. Indeed, we claim in the article that the simulation shows this 'top-down' evolution likely because there is no wind shear at the top of the boundary layer to maintain the production of turbulence. In the observations, the directional wind shear at the top of the BL might have maintained the production of turbulence in the upper layers, so that the 'top-down' process might be reduced. We can not confirm the 'top-down' process with aircraft data but the temporal evolution of the TKE dissipation rate obtained from the UHF on 20 June 2011 (see Figure 3) reveals a slight 'top-down' process, less pronounced than in the simulation, which is consistent with the presence of more important shear at the top of the BL.

Figure 2: Temporal evolution of the volume averaged TKE over the boundary layer depth from (a) Rizza et al. (2013) and (b) Nadeau et al. (2011).
“In this study, the simulation shows this top-down evolution likely because the shear in wind direction at the top of the boundary layer is weak and does not maintain the dynamical turbulence production. We can expect a reduced top-down effect in the reality since there is shear in direction which is not simulated.”

Figure 3: Temporal evolution of the TKE dissipation rate obtained from the UHF on 20 June 2011. Two estimates of $z_i$ from lidar and UHF are also represented by white symbols.

Regarding the formal aspect of the manuscript; (i) the references, especially in the introduction are not really exhaustive, there are recent works that are not mentioned at all and (ii) the description of LES model is quite concise: which SFS modeling and geostrophic forcing ????

The revised manuscript includes a larger bibliography and more description of the LES model. These points will be discussed later in the specific comments. We thank the reviewer for the references suggestions.

SPECIFIC COMMENTS

pag.32494, line 10 There are recent works that should be mentioned, among the others:

pag.32494, line 13 I would mention also the analytical studies of: A.G. Goulart, G.A. Degrazia, -

pag.32494, line 25 I would add: Rizza et al (doi:10.1016/j.physa.2013.05.009) as 2013b

These references have been included in the revised manuscript. As already mentioned above, the discussion concerning the TKE decay has been enlarged in order to better articulate our study among the previous ones.
In addition to this, we have referred to Goulart et al. (2010) several times in the revised manuscript.

**Pag.32497, line 20 Please explain acronyms Ibimet and Isafom**

These acronyms have been defined in the revised manuscript.

**Pag.32499 - chapter 3 LES - Which SFS model have been used? the standard NCAR code use:**


The following sentence has been added in the revised version in section 3.1, l. 283:

“The subgrid-scale model includes a turbulent-kinetic-energy eddy-viscosity model suggested by Deardorff (1980), used by Moeng et al. (1984) and improved by Sullivan et al. (1994).”

- The NCAR-LES code use the geostrophic wind as a surrogate of the large-scale horizontal pressure gradient, please comment which value is being used.

Reviewer 1 pointed out an important information that was not clearly given in the manuscript. We did not prescribe any geostrophic wind. We simply initialize the simulation with a vertical wind profile obtained from a simplified 0515 UTC radiosounding, and let it evolve without any forcing. Consequently, the simulation is not able to reproduce the change of wind direction that is visible in the observations.

We have clarified this in the text in section 3.1, l. 304:

“The wind, potential temperature and specific humidity initial profiles were deduced from the 0515 UTC radiosounding (see dashed lines in Fig. 2 for temperature and wind speed). No geostrophic wind is prescribed. This simple representation of the wind leads to a simulation with very low wind speed as it is the case in the observations, but does not allow to simulate the shear in wind direction.”

**Pag.32500 – line 15 What “simplified” does it mean exactly ???**

The wind and potential temperature profiles have been added on Figure 2 (in black dashed lines) in the revised paper and show approximately two distinct layers.

In the revised manuscript, we have better introduced the initial profiles and Fig 2, in section 3.1, l. 304:

“The wind, potential temperature and specific humidity initial profiles were deduced from the 0515 UTC radiosounding (see dashed lines in Fig. 2 for temperature and wind speed).”

**Pag.32500 – lines 19-23 Concerning the large-scale advectons, why (u,v) predictions from AROME model are not used ?? ??**

As we already mentioned earlier, the goal of the simulation was not to simulate a real case in its whole complexity, but rather to build a reasonable mean BL structure, that is close enough to the observed structure, in order to analyze what turbulence structure evolution would be built in the LES. We did not find appropriate to prescribe wind advection with such an idealized wind profile.

We better explained our goal in Section 3, l. 265:

“Our aim is not to reproduce a real case but rather to use the BLLAST dataset as a benchmark to simulate a boundary layer with the same range of thermal and dynamical instabilities than the one observed during BLLAST.”

**Pag.32500 – chapter 3.2 - Figure 4 is a bit confusing, please use less profiles with a different choice of colors (red-blue-black) and thicker lines. I think that there are significant differences between LES and OBS profiles for all variables, especially for the wind speed. For example for the 1800 UTC (yellow line) profile, the observed wind speed at 1100 m is almost zero while the LES prediction is 6 ms⁻¹, while at the same hour the DT (LES-OBS) is almost 3K. Furthermore it would be interesting to see a zoomed view of WS in the first 100m. - The LES vertical domain is 3072 m while the figures are up to 2000m.”
Figure 4 of the manuscript has been changed. The new Figure 4 in the revised manuscript shows less profiles (at 0530, 1130, 1330, 1730 UTC), with different colors. Since we focus on the PBL evolution and not on what happens far above, the chosen representation is a compromise in order to see correctly both the first 100 m and the entire PBL. Figures 4 and 5 show the zoomed and un-zoomed view of the figure 4. We do not think it is worth to add these figures in the revised manuscript, since for our purpose, there is no specific need to show the profiles above 2000 m.

In the boundary layer, the evolution of $\theta$ is well reproduced. At 1100m, the 3K difference between the LES and the radiosounding at the top of the boundary layer is rather explained by a $z_i$ departure rather than a departure in $\theta$ in the BL.

At 1800 UTC, the observed wind speed at 1100m is almost zero due to the directional wind shear at the top of the PBL, which is not reproduced in the simulation.

Close to surface, we do not expect the simulation to reproduce perfectly well the observations, since we compare an idealized surface relatively to a complex real surface. In the first 100 m:
- The differences of wind are small: the wind speed is weak (between 2 and 4 m/s in the PBL) in both observations and LES.
- The differences of super-adiabatism at 1130UTC might be due to the different location from where the radiosounding was launched, which might be warmer than the moor surface. Moreover, the stronger wind shear might explain why the suradiabatic layer seems thicker in the observations. The difference in stability timing observed on the 1730 UTC profiles are also discussed in the revised version.

More discussion has been included in the revised paper, in section 3.2, l.353:

"In the first 100 m, the differences of stability profile at 1130 UTC might be due to the different locations of the soundings and the moor site where the surface flux is observed. The 1730 UTC LES profile is already neutral, whereas the observations at 1750 UTC still show super-adiabatism. The differences are due to the fact that as soon as the surface buoyancy fluxes turn negative, the LES potential temperature profile becomes stable at the lower layers of the BL. This delay between the time when the buoyancy flux goes to zero and the time when the local gradient of virtual potential temperature changes sign has been observed and analyzed in Blay et al. (2014). It can be of the order of 30 min or 1 hour."
Figure 4: Zoom of the first 500 m of the vertical profiles of $\theta$, $r$, wind speed (WS) and wind direction (WD) observed (solid lines and dotted lines for WD) and obtained by LES (dashed lines).

Figure 5: Un-zoomed view of the vertical profiles of $\theta$, $r$, wind speed (WS) and wind direction (WD) observed (solid lines and dotted lines for WD) and obtained by LES (dashed lines).
Discussion about zi and differences between LES and observations, as well as a proposition of explanation were already made in lines 26-31. So we did not understand the Reviewer's comment.

After 1800 UTC zi (RS-UHF) is almost 1100 m, while LES prediction is 800 m. Anyway, after 1800 UTC the surface heat flux should have reversed its sign and the PBL should be under stable conditions. Is it realistic ??? I think that authors should provide also a description of stability conditions, perhaps introducing the Richardson number and/or the MO length/velocity scales (L, ustar). These surface parameters are important because in the following it is introduced the concept of delay time between the surface and upper TKE. In these conditions it is important to verify that surface parameters are well reproduced by the simulation.

Due to the difficulty for the LES to run in stable conditions, we did not wish to study the LES results once the fluxes get to zero, or at least, one must take very cautiously those results and the comparison between LES and observation after that time (1800 UTC). Moreover, as soon as the surface fluxes turn negative, the LES potential temperature profile indeed turns immediately to stable at the lower levels, whereas a delay around ~ 30-80 min between the time when the buoyancy flux goes to zero and the time when the local gradient of virtual potential temperature indicates a sign change may be observed, as shown by Blay et al. (2014). The LES is not able to reproduce this delay and it was not the purpose of this study.

Our focus is on the evolution during the decrease of the positive flux. We show in Figure 6 the comparison of the thermal and dynamical instability for both LES and observations during this period. u* and θ* are calculated from Monin Obukov theory in LES. The dynamical and thermal instabilities are very similar in the simulation and in the observations. A comment about the similar dynamical and thermal instabilities in the simulation and observations has been added in section 3.2, l. 438:

“In summary, the simulated boundary layer is comparable to the observed one in terms of boundary layer height, wind speed, and dynamical and thermal stability (not shown) near the surface.”
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Below there is a copy of the reviewer 2 comments (in italic and blue), with a detailed response to each points.

Responses to Reviewer 2:

This paper concerns an LES of the afternoon transitional boundary layer, focusing particularly on the spectral characteristics of the decaying convective turbulence. The simulation is based on a well-observed field experiment and comparisons with the observations are included. It is a useful addition to the literature on the BLLAST experiment and on transitional boundary layers more generally. My comments are mainly requests for small clarifications, but, more substantively, I think that additional discussion of the budget of TKE, shown in Fig. 6, would be useful.

1. p. 32498, L. 16. Does advection here include subsidence

Yes, we prescribed total advection, which includes horizontal and vertical (due to subsidence) advection.

2. p. 32499, L. 14. What is the height of the flux measurements over the individual surface types? Does the 60m tower have a large enough footprint to give a domain average, even in the most unstable cases, or is the predominance of the moor surface type the key point?

The flux measurements were made between 2 and 5 m over the different surfaces, depending on the vegetation height (see Lothon et al. 2014).

We think that the 60m mast measurements are representative of the region except for some wind directions: for instance in case of south west winds, the measurements might not be representative because a large forest has then more influence in the measured flux (see a study on area averaged flux in http://bllast.sedoo.fr/workshops/february2015/presentations/Hartogensis-Oscar_area-averaged-flux.pdf).
Besides, about 40% of the plateau is covered by moor and grasslands (very similar types of surfaces), which make the moor fluxes the most representative of the region.

In the revised manuscript, we have specified the reason why we consider the moor vegetation as the dominant vegetation over the plateau, in section 2.2, I.240:

“As such, H measured at 60 m height is encompassed in all the others and is close to the moor and grass, the dominant vegetation, representing about 40% of the covers over the plateau.”

3. p. 32499, L. 15. Do you necessarily expect the latent heat flux to reach 0

In case of larger surface wind speed, we could have expected the latent heat flux not to be zero, but during the BLLAST campaign low surface winds were observed and consequently, almost zero latent heat flux. However we wrote the sentence in a more general way:

“This delay is observed for all the intense observation periods (IOP) of the BLLAST campaign implying that the latent heat flux reaches its minimum value systematically later than the sensible heat flux.”

4. p. 32500, L. 1. The boundary conditions need to be described more prominently. I think moving the sentence "A simulation is initialized...advection." to the top of section 3.1 and adding "observed surface heat flux at the moor site" would make this more obvious. The sentence on lines 17 and 18 of this page could then be removed.

The suggestion to specify the boundary conditions in the beginning of the paragraph has been taken into account in the revised manuscript. We also realized that we forgot to mention that the lateral conditions are cyclic. The new paragraph in section 3.1, l. 273 is:

“Our LES is initialized with early morning radiosoundings and forced with homogeneous surface fluxes, based on those measured over the moor surface. Temperature and humidity advection are prescribed. The side wall boundary conditions are periodic.

The LES code from National Center for Atmospheric Research (Moeng (1984), Sullivan and Patton (2011), Patton et al. (2005), Lohou and Patton (2014)) is based on the Boussinesq equations, including conservation laws for momentum, mass and the first law of thermodynamics.”

5. p. 32502, L.3. It would be interesting to relate Fig. 6 to the budget of TKE, including production, shear etc., to explain why the region of negative buoyancy is deeper. Perhaps figures of the non-dimensional budgets at the start of the AT, at the end of the first phase and at the end of the second phase would be useful. As the authors note, in the real atmosphere there was more shear at the top of the BL, so their idealization will underestimate entrainment, but it should be conceptually helpful in understanding the decay of convective turbulence.

This is a very good remark and we did verify before the submission of this paper if the TKE budget could help us to understand these two steps in the TKE decrease and the demixing height evolution. As you can see in Figure 1, whereas all the TKE budget terms decrease during the AT (left panel), their respective contribution to the TKE tendency is not evolving significantly and can explain neither the negative layer deepening nor the two stages of the TKE tendency. From our point of view the demixing and TKE decay processes are scale dependent and cannot be seen on statistical moments.

Without adding any figures in the text we introduced a comment on the TKE budget in the discussion, section 5.4, l.825:

“ The TKE budget evolution in time was of any help to explain the two stages of the TKE decrease. Whilst the different terms do decrease with time, their respective
contribution to the TKE tendency hardly change from the first to the second stages (not shown).

Figure 1: 30-min averaged TKE budget terms normalized (left panel) and not normalized (right panel) at 12:00, 16:00 and 17:00 UTC (thin, thick and dashed lines, respectively). “bp”, “mp”, “diss” and “res” stand for the buoyancy production, the mechanical production, the dissipation and the residual term which should correspond to the transport.

6. p. 32503, L. 13. This paragraph is confusing: "Despite...nevertheless...Despite". It’s not clear whether you think the LES is good enough or not. Please be more specific about which aspects of the LES are expected to be realistic and where caution is appropriate.

We totally agree that this sentence was not clear. We have reformulated this sentence in the revised manuscript, in section 3.2, l. 437:

“In summary, the simulated boundary layer is comparable to the observed one in terms of boundary layer height, wind speed, and dynamical and thermal stability near the surface. The lower development of the PBL height of about 200 m and the underestimated TKE by a factor of 1.5 can be explained by the directional wind shear which is not simulated. The latter might increase the entrainment and the turbulence dynamical production at the top of the boundary layer. Despite these differences on the main PBL structure, the simulation is realistic enough to evaluate how the turbulence evolves in a convective boundary layer during the AT and the comparison of simulated and observed boundary layer will be analyzed accordingly.”

7. p. 32506, Eq. 16. I wondered whether a weighting with SKL89(k) would improve the measure, so as not to overemphasise noise in weaker parts of the spectrum.

From this suggestion, we have investigated the temporal evolution of the index of quality, by weighting the KL89 analytical spectral model. The formula becomes:
\[ IQ_{\text{weighting}} = \sum_k \left( \frac{S_{KL89}(k)}{S_{KL89}(k)} \log \left( \frac{S_{OBS}(k)}{S_{KL89}(k)} \right) \right) \frac{1}{\sum_k S_{KL89}(k)} \]

Figure 2 shows the temporal evolution of \( IQ_{\text{weighting}} \). This weighting does not improve neither the tendency nor the intensity of the error and does not help to better detect the poorest fits. Considering that, we kept our definition of \( IQ \).

Figure 2: Temporal evolution of the quality index with (dashed lines) and without (continuous lines) weighting of the KL89 analytical spectra.

8. p. 32507, L. 19. I was confused here. Fig. 8 shows higher values of \( k \) at 18:00 UTC, implying shorter wavelengths, yet you say \( \Lambda \) increases. Yes, it was indeed a mistake in our written comment of those figures. Figure 3 represents the temporal evolution of \( \Lambda \) from LES and aircraft observations. \( \Lambda \) slightly increases until 1630 UTC then decreases. With the simple concept that \( \Lambda \) represents the distance between two structures and \( l_w \) represents the width of a structure, this means that during the LAT, the thermals become closer from each others whereas the increase of \( l_w \) means the thermals become larger. This is consistent with a decreasing skewness of \( w \) as time evolves, which we do find in both observation and LES.

We have corrected the article and added this discussion in the revised manuscript in section 5.2.3, L. 731:

“As noticed in Fig. 8, \( \Lambda_w \) drifts slightly toward smaller eddies. Keeping in mind that \( \Lambda_w \) represents the distance between two structures and \( l_w \) represents the width of a structure, this means that during the LAT, the thermals become closer from each others whereas the increase of \( l_w \) means the thermals become larger. This is consistent with a decreasing skewness of \( w \) as time evolves, which we do find in both observation and LES (not shown).”
9. p. 32508, L. 9. Do you mean "decay of TKE" rather than "decay of TKE dissipation rates"?

No we do not. It is the decay of TKE dissipation rate that we are talking about.

10. p. 32509, L. 13. An explanation of why anisotropy or coherent structures could explain this is needed.

Theoretically, a fundamental hypothesis for the -2/3 slope in the inertial subrange slope for $kS(k)$ is isotropic turbulence. So one may wonder if this slope remains at -2/3 for anisotropic fields.

We have added the following discussion in the revised manuscript in section 5.2.1, l. 665:

“Theoretical -2/3 slope is based on the hypothesis of isotropic turbulence. Therefore, a possible explanation for these steeper slopes in convective conditions could be the loss of isotropy in real conditions and in particular the role of convective structures and the associated anisotropy. As mentioned before, in section 5.1, they are responsible for anisotropy smaller than one. We believe that the more ‘coherent’ or organized the $w$ field, the smaller the anisotropy and the steeper the slope. But this explanation needs further work for confirmation.”

Note that in this KL89 analytical spectrum, anisotropy of turbulence is taken into account only by varying integral scale from transverse to lateral spectra. Even considering anisotropy, the spectrum follows the usual -5/3 slope in the inertial subrange.

This comment has been included in the revised manuscript.

11. p. 32510, L. 23. Define LAT

This acronym has been defined in the revised manuscript.

Figure 3: Temporal evolution of $\Lambda$ observed (open circles) and obtained by LES (continuous lines) at different heights (same color code than for other figures).
12. p. 32511, L. 18. Does the decrease actually propagate, or does is it simply that surface-driven turbulence does not rise so high?

This is a good point that has been clarified in the manuscript. We agree that “propagates” is probably not the most appropriate word to explain this, and that it is more that surface-driven turbulence does not rise so high. Since the surface fluxes decrease during the afternoon transition, the turbulence produced at surface does not reach the top of the CBL anymore. Since there is also no dynamical production at the top of the PBL in our case, this induces that turbulence decreases first at the top of the PBL whereas it is maintained longer at surface.

We have modified the revised article accordingly in section 5.3, l.754:

“That is, once the surface flux starts to decrease, the surface-driven turbulence does not rise up to the top of the CBL anymore. This induces that turbulence decreases first at the top of the PBL whereas it is maintained longer under 0.15 z.”
Turbulence vertical structure of the boundary layer during the afternoon transition

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Abstract. We investigate the decay of planetary boundary layer (PBL) turbulence in the afternoon, from the time the surface buoyancy flux starts to decrease until sunset. Dense observations of mean and turbulent parameters were acquired during the Boundary Layer Late Afternoon and Sunset Turbulence (BLLAST) field experiment by several meteorological surface stations, sounding balloons, radars, lidars, and two aircraft flying extensively during the afternoon transition. We analyzed a case study based on some of those observations and Large-Eddy Simulation (LES) data focusing on the turbulent vertical structure throughout the afternoon transition.

The decay of turbulence is quantified through the temporal and vertical evolution of (1) the turbulence kinetic energy (TKE), (2) the characteristic length scales of turbulence, (3) the shape of the turbulence spectra. A spectral analysis of LES data, airborne and surface measurements is performed in order to characterize the variation of the turbulent decay with height and study the distribution of turbulence over eddy size.

This study points out the LES ability to reproduce the turbulence evolution throughout the afternoon. LES and observations agree that the afternoon transition can be divided in two phases: (1) a first phase during which the TKE decays with a low rate, with no significant change in turbulence characteristics, (2) a second phase characterized by a larger TKE decay rate and a change in spectral shape, implying an evolution of eddy size distribution and energy cascade from low to high wavenumber.

The changes observed either on TKE decay (during the first phase) or on the vertical wind spectra shape (during the second phase of the afternoon transition) occur first in the upper region of the PBL. The higher within the PBL, the stronger the spectra shape changes.

1 Introduction

The transition from a well-mixed convective boundary layer to a residual layer overlying a stable nocturnal layer raises several issues (Lothon et al., 2014), which remain difficult to address from both modeling and observational perspectives. The well mixed convective boundary layer with fully developed turbulence is mainly forced by buoyancy. The afternoon decrease of the surface buoyancy flux leads to the decay of the turbulence kinetic energy (TKE), and a change of the structure of the turbulence, which shows more anisotropy and intermittency. It is important to better understand the processes involved, as they can influence the dispersion of tracers in the atmosphere (e.g., Vilà-Guerau de Arellano et al., 2004; Casso-Torralba et al., 2008; Carvalho et al., 2010; Taylor et al., 2014), and the development of the nocturnal and daytime boundary layers of the following days (Blay-Carreras et al., 2014b).
Turbulence decay has been studied with laboratory experiments (e.g., Monin and Yaglom, 1975; Cole and Fernando, 1998), theoretical models (Goulart et al., 2003), numerical studies with Large-Eddy Simulations (LES) (e.g., Nieuwstadt and Brost, 1986; Sorbjan, 1997; Rizza et al., 2013a) and observations (e.g., Fitzjarrald et al., 2004; Grant, 1997; Brazel et al., 2005; Fernando et al., 2004). In all of those studies, the decay was mainly related to the decrease of the surface buoyancy flux, but with complexity gained with shear-driven boundary layers (Pino et al., 2006; Goulart et al., 2010), which slow the decay. Using LES, Nieuwstadt and Brost (1986) considered a sudden shut off of surface heat flux, and found that turbulence decay occurred within a period of the order of the convective time scale $t_c = z_i/w_∗$, where $z_i$ is the planetary boundary layer (PBL) depth, and $w_*$ is the convective velocity scale (Deardorff, 1970). However, different results were obtained if a slower decrease of the forcing surface buoyancy flux is considered with an external time scale $τ_f$ (Sorbjan, 1997; Rizza et al., 2013a,b; Nadeau et al., 2011). If $τ_f$ is large relative to $t_c$, the turbulence can adjust to the forcing change, in quasi-equilibrium, as noted by Cole and Fernando (1998). This is the case in the mid-afternoon PBL, when $t_c$ is around 10 or 15 min and $τ_f$ is around 2 or 3 h. Sorbjan (1997) found that the TKE decay scales with $τ_f/t_c$, with $t_c$ estimated at the start of the decay. But in late afternoon and sunset, $t_c$ starts to increase significantly (until the definition of $w_*$ is put into question at zero buoyancy flux), and turbulence may not be able to adjust to the external change. Consequently, an extensive description of the turbulence structure is needed to better understand this decay process in the PBL.

The evolution of the turbulence length scales across the AT has not been addressed extensively, but several studies can be found obtaining diverging results. With fundamental consideration of eddy lifetime, or “turn over” time scale, one may state that smaller eddies will decay earlier than larger eddies (Davidson, 2004). This is one explanation given by Sorbjan (1997), from an LES study, for the increase of the characteristic length scale of the vertical velocity found in the mixed (then residual) layer of the LES. In the surface layer, one may expect the length scales to decrease, as inferred by Kaimal et al. (1972) from the study of surface-layer spectra evolution with stability during the Kansas experiment. With tethered-balloon observations, Grant (1997) indeed showed that the peak of the vertical velocity spectra shifts to smaller length scales in the surface layer during the evening transition. Finally, Nieuwstadt and Brost (1986) and Pino et al. (2006) found that the length scale of maximum spectral energy of the vertical velocity remained constant during the decay process. By using a theoretical model of the TKE spectrum and LES, Goulart et al. (2010) have also found that the spectral peak remains at approximately the same wavelength when shear is strong enough to prevent the spectral peak of vertical velocity from shifting towards shorter wavelengths. For other meteorological variables such as the horizontal wind components, temperature and moisture, Pino et al. (2006) have shown that the characteristic length scales increase with time.

The evolution of the turbulence scales remain unclear and only partly understood. It must be thoroughly investigated whether the scales in the mixed and afterward residual layer really increase or not. Considering the time response and equilibrium aspect mentioned above, and the possible decoupling with height between the stabilizing surface layer and the overlying residual layer, it is also important to consider the vertical structure of turbulence decay, i.e. the evolution of turbulence and scales as a function of height. Except Goulart et al. (2010), the numerical studies quoted before (e.g., Sorbjan, 1997; Pino et al., 2006) considered TKE integrated over the entire PBL depth, and observations of the turbulence decay were made most of the time at surface (Nadeau et al., 2011). Only few observational studies considered the vertical structure of the turbulence afternoon decay (Grant (1997), Fitzjarrald et al. (2004) in the afternoon-decaying PBL).

Here we investigate the evolution of the turbulence spectra and scales from surface to CBL top during the afternoon transition (AT) based on the BLLAST (Boundary Layer Late Afternoon and Sunset Turbulence) dataset, collected during summer 2011 (Lothon et al., 2014). A cloud-free, weak wind day (20 June 2011) is considered to analyze the evolution of the turbulence, from midday to sunset, by using both observations and an LES model. Our analysis aims at (1) evaluating with a complete observations data set the capabilities of the LES to simulate the turbulence structure of the afternoon decay, (2) analyzing the evolution of integral scales, TKE, shape of the spectra in both observations and numerical simulation, and as a function of height.

The article is organized as followed: In the next Section, we present the experimental dataset and describe the case study of the 20 June 2011 through the observations (Section 2). In Section 3, the LES is presented and evaluated with the observations. Our spectral analysis method, used in both observations and LES, is then described in Section 4, before we present and discuss our results (Section 5). Concluding remarks are given in Section 6.

2 Experimental dataset and case study

The BLLAST experiment took place in the south of France, near the Pyrénées mountain range, during the summer 2011. A set of various observational platforms (aircraft, Remotely Piloted Aircraft Systems, balloons) and continuous measurements (towers, remote sensing) monitored the PBL diurnal evolution, focusing on the AT, in various meteorological regimes. BLLAST experiment provides a unique dataset to investigate the vertical structure of the decaying PBL (see Lothon et al. (2014) for a detailed description of BLLAST objectives and experiment).
The experimental dataset used in this study, the chosen study case and its simulation are now described. Note that the site longitude is around 0.21°E, consequently UTC, very similar to local solar time, is used hereafter as the time reference.

### 2.1 Experimental dataset

In order to monitor the evolution of the mean structure of the PBL during the AT (and initialize the simulation), we use standard radiosoundings launched every 6 hours, from 0600 UTC to 1800 UTC, and hourly radiosoundings (Legain et al., 2013) of the low troposphere (up to 3 to 4 km), from 1300 to 1800 UTC. The launching sites of the two types of radiosoundings are 4 km apart. The radiosondes measured temperature, water vapour content and the sonde location from which the horizontal wind components are deduced.

Surface energy balance and turbulence structure in the surface layer are provided by several ground stations over different vegetation coverages (wheat, corn, grass, pine forest and moor (composed of heather and gorse)). A permanent 60 m tower provides integrated turbulence measurements in the surface layer above the heterogeneous surface. The statistical moments are estimated over detrended 30 min periods from 10 Hz raw measurements. The surface heat fluxes are used as surface forcing in the simulation.

Two aircraft, the French Piper Aztec (PA) from SAFIRE (Service des Avions Franc¸ais Instrument´es pour la Recherche en Environnement) (Sa¨ıd et al., 2005) and the Italian Sky Arrow (SA) from Ibitem (Istituto di Biometeo- rologia del CNR) and Isafom (Istituto per i Sistemi Agricoli e Forestali del Mediterraneo) (Gioli et al., 2006), flew extensively during the afternoon, at 65 m s\(^{-1}\) and 40 m s\(^{-1}\), respectively. They measured temperature, moisture, pressure, CO\(_2\) mixing ratio and 3-D wind at 50 Hz (SA) and 25 Hz (PA) along 25 to 40 km legs stabilized in attitude and altitude. The detailed instrumentation of both aircraft is given in Lothon et al. (2014).

### 2.2 Case description

20 June 2011 was selected as our case study on the basis of meteorological criteria and data coverage. The synoptic situation was a high pressure system over South-West of France, with a light westerly wind leading to a fair and cloud-free weather.

Figure 1 gives the normalized altitude \(z/z_i\) of the stacked legs flown by the aircraft as well as the different launching times of the radiosoundings (the method used for the PBL height \(z_i\) estimation is discussed later). The two aircraft flew simultaneously, the PA flying above the SA. They flew along west-east parallel legs, at three latitudes and, as shown in Fig. 1, at six heights within the PBL, and two different time periods: the first one from 1430 UTC to 1530 UTC, the second one later, from 1745 UTC to 1900 UTC. This flight strategy gives access to six heights to study the vertical structure of the turbulence within the PBL.

Figure 2 presents the evolution of the potential temperature \((\theta)\) and the wind direction in the PBL at several hours from 0500 to 1800 UTC on 20 June 2011. During the day, the PBL warms by about 7 K and the PBL depth \(z_i\) grows up to about 1100 m above ground level. Figure 2a also reveals a warm advection above the PBL between 0515 UTC and 1100 UTC that must be taken into account when simulating. After 1100 UTC, the \(\theta\) profile hardly changes in the free atmosphere, meaning that the temperature advection is very weak.

Figure 2b shows an easterly wind within the PBL, veering to westerly above. The wind intensity remains constant all along the day (not shown): it is weak within the PBL (less than 4 m s\(^{-1}\)) and increases with height, up to 10 m s\(^{-1}\) at 1500 m.

The water vapour mixing ratio \((r)\) increases from 8 to 10 g kg\(^{-1}\) in the PBL until 1300 UTC and decreases afterward. The temporal evolution of the PBL mean vertical structure is further analysed in section 3.2.

The surface sensible and latent heat fluxes (H and LE, respectively) measured above various vegetation coverages are presented in Fig. 3. The maximum value of H varies from 100-130 W m\(^{-2}\) over grass and moor to 450 W m\(^{-2}\) over the pine forest. LE shows much less variability between vegetation coverages, maximum values varying from 250 W m\(^{-2}\) to 350 W m\(^{-2}\). The measurements at 60 m height integrate a large footprint and should give flux estimates of the heterogeneous landscape. As such, H measured at 60 m height is encompassed in all the others and is close to the moor and grass, the dominant vegetation, which represents about 40% of the vegetation cover over the plateau.

In this study, the AT is defined as the period from the time when the surface buoyancy flux is maximum, to the time where it goes to zero (the surface buoyancy flux is defined as the turbulent vertical transport of virtual potential temperature and is approximated as a linear combination of observed surface sensible and latent heat flux). This period varies according to the surface (Lothon et al., 2014). For the moor coverage, whose surface fluxes will be used to drive the simulation of the 20 June 2011, this period starts at 1200 UTC and ends at 1750 UTC, while it ends 20 minutes earlier when considering H instead of the buoyancy flux. This delay is observed for all the intense observation period (IOP) days of the BLLAST campaign implying that the latent heat flux reaches its minimum value systematically later than the sensible heat flux. Thus the forcing time scale of the surface flux decay \(\tau_f\) is around 5.8 hours over the moor surface.

### 3 LES

As a complementary tool, a LES is initialized with the BLLAST observations to study turbulence decay of convect-
tive boundary layer over an homogeneous and flat surface. The observations of the 20 June are used to guide our simulation, like the 1 July and 25 June guided the studies of Blay-Carreras et al. (2014b) and Pietersen et al. (2015) respectively. Our aim is not to reproduce a real case but rather to use the BLLAST dataset as a benchmark to simulate a boundary layer with the same range of thermal and dynamical instabilities than those observed during BLLAST.

### 3.1 LES configuration and initialization

Our LES is initialized with early morning radiosoundings and forced with homogeneous surface fluxes, based on those measured over the moor surface. Temperature and humidity advection are prescribed. The side wall boundary conditions are periodic.


The simulation resolves a domain of \(10.24 \times 10.24 \text{ km}^2\) horizontally and 3.072 km vertically, with \(\Delta x = \Delta y = 40 \text{ m}\) and \(\Delta z = 12 \text{ m}\) of horizontal and vertical resolution, respectively. This results from a compromise between the computation time and three constraints: (1) the domain size and resolution were chosen after a sensitivity study (not shown) so that the LES spectra were able to represent the main characteristics of the observed spectra, (2) the resolution was chosen so that the ratio of \(z_1\) to \((\Delta x \times \Delta y \times \Delta z)^{1/3}\) was large enough to ensure that the results are independent of the resolution (Sullivan and Patton, 2011), and, (3) the ratio of \(\Delta x\) to \(\Delta z\) was kept rather small, but with a high enough vertical resolution to correctly represent the entrainment zone (Sullivan and Patton, 2011). The time step evolves during the simulation and is about 1.4 s for fully convective conditions.

The simulation was initialized early in the morning, in order to ensure a fully turbulent convective PBL by the afternoon. The wind, potential temperature and specific humidity initial profiles for the LES were deduced from the 0515 UTC radiosounding (see dashed lines in Fig. 2 for temperature and wind speed). No geostrophic wind is prescribed. This simple representation of the wind leads to a simulation with very low wind speed as it is the case in the observations, but does not allow to simulate the shear in wind direction. An homogenous and flat surface is considered in the LES with imposed surface fluxes which are those measured at the moor site (Fig. 3).

Vertical profiles of large-scale total advections (horizontal plus vertical advection) of heat and moisture were hourly prescribed in the simulation and linearly interpolated in between. They were derived from AROME forecast model (horizontal resolution of 2.5 km), using the 16 grid points in a box surrounding the experimental site. This model confirms predominant zonal advection, especially during the morning.

From 0515 UTC to 1000 UTC, the temperature advection is important and about \(10 \text{ K day}^{-1}\) from 500 m up to 1500 m (not shown). After 1100 UTC, it decreases and is negligible in the afternoon. This is consistent with what is observed on the evolution of the potential temperature (Fig. 2a). From sunrise to 1400 UTC, the moisture advection is about \(-10 \text{ g kg}^{-1} \text{ day}^{-1}\) from the surface up to 500 m, and about \(-10 \text{ g kg}^{-1} \text{ day}^{-1}\) above. After 1400 UTC, the moisture advection weakens (not shown).

The data files used to run this case (initial profiles, surface flux and advection profiles) are available on the website of the BLLAST database (http://bllast.sedoo.fr/database).

### 3.2 Evaluation of the simulated boundary layer

The bracket notation \(\langle \psi \rangle\) for any simulated variable \(\psi\) is used to represent the 2D-horizontal average over the LES domain. The same notation is used for the 1D-horizontal average of the airborne measurements along the legs. For the surface dataset, \(\psi\) represents the time average notation. For these three types of datasets, the turbulent fluctuations \(\psi'\) are defined as deviations from the corresponding mean. For a more fair comparison with the simulated variances, the observed variances are estimated by integration of the spectra over a horizontal and temporal average.

The evolution of the simulated \(\theta\) vertical profiles is compared with observations in Fig. 4a from 0530 to 1750 UTC. The simulated \(\theta\) is close to the observations in the mixed layer (differences lower than 0.1 K) and in the free atmosphere, simulating the change in \(\theta\) profile between 0515 UTC and 1115 UTC due to the prescribed advection.

In the first 100 m, the differences of stability profile at 1130 UTC might be due to the different locations of the soundings and the moor site where the surface flux is observed. The 1730 UTC LES profile is already neutral, whereas the observations at 1750 UTC still show superadiabatism. The differences are due to the fact that as soon as the surface buoyancy fluxes turn negative, the LES potential temperature profile becomes stable at the lower layers of the BL. This delay between the time when the buoyancy flux goes to zero and the time when the local gradient of virtual potential temperature changes sign has been observed and analyzed in (Blay-Carreras et al., 2014a). It can be of the order of 30 min or 1 hour.

Figure 4b presents the evolution of the water vapour mixing ratio. The temporal evolution of \(r\) profiles shows a well
simulated daily humidification. One can notice a 1 g kg\(^{-1}\) departure at 1305 and 1750 UTC than actually observed.

The horizontal mean wind speed is well reproduced in the simulation during the day: the wind remains weak and about 2 m s\(^{-1}\) in the PBL. \(u_w\) evolves from 0.2 to 0.1 during the afternoon for both observed and simulated data. The wind increases with altitude above the PBL and reaches 10 m s\(^{-1}\) at 2000 m. No wind forcing is prescribed in the simulation, therefore the observed wind direction change from West to East within the mixed layer between 0530 and 1130 UTC is not simulated (Fig. 4d). Whilst the wind speed shear is well simulated, the wind direction shear is evidently underestimated. Consequently, shear-driven processes (Pino et al., 2006) might not be as important in the simulation as in the observations.

The simulated vertical profiles of the buoyancy flux normalized by the surface buoyancy flux at the start of the AT (Fig. 5) have a quite classical shape until 1330 UTC with a linear decrease with height and negative flux above 0.8 \(z_i\). In the simulation, \(z_i\) is estimated as the height of the mixed layer, determined with a threshold on the certainty of \(z_i\) the previous day. After 1000 UTC, \(z_i\) is estimated as the altitude of the maximum relative humidity between 0530 and 1130 UTC is not simulated (Fig. 4d). Whilst the wind speed shear is well simulated, the wind direction shear is evidently underestimated. Consequently, shear-driven processes (Pino et al., 2006) might not be as important in the simulation as in the observations.

The simulated vertical profiles of the buoyancy flux normalized by the surface buoyancy flux at the start of the AT (Fig. 5) have a quite classical shape until 1330 UTC with a linear decrease with height and negative flux above 0.8 \(z_i\). In the simulation, \(z_i\) is estimated as the height of the mixed layer, determined with a threshold on the \(\theta\) vertical gradient (0.01 K m\(^{-1}\)). This method was preferred to the one used for radiosoundings (see below) because of the complex humidity profiles which lead to more fluctuating \(z_i\) estimates. However, the difference between these two estimates is less than 50 m. After 1330 UTC, the upper layer characterized by negative entrainment flux deepens and goes down to 0.6 \(z_i\) at 1800 UTC. During the AT the entrainment rate (ratio of the buoyancy flux at the top of the PBL to the buoyancy flux at surface) remains constant and about -0.13 (not shown). Unfortunately, this value cannot be compared to observations since the fluxes deduced from airbornemeasurements in the PBL vary substantially at that time, and because of lack of statistics of the large scales in a less and less stationary PBL. Long enough aircraft legs to get accurate statistical moment estimates in convective PBL (Lenschow et al., 1994) are even more relevant during the AT.

The temporal evolution of \(z_i\) has been estimated from Ultra High Frequency radar wind profiler (hereafter UHF) and radiosounding measurements and compared to the simulation (Fig. 6). \(z_i\) is estimated from UHF as the maximum of the refractive index structure coefficient (Heo et al., 2003; Jacoby-Koaly et al., 2002). From radiosoundings, \(z_i\) is estimated as the altitude of the maximum relative humidity below 2500 m (this criterion has been shown to be consistent in time and height during BLLAST experiment (Lothon et al., 2014)).

Until 0900 UTC, the UHF detects the residual layer of the previous day. After 1000 UTC, \(z_i\) increase is similarly depicted by the UHF and radiosoundings, with a maximum value of 1100 m. The simulated PBL grows slower than the observed PBL and reaches 850 m. This discrepancy between observed and simulated \(z_i\) (which is larger than the uncertainty of \(z_i\) estimate) might be partly explained by a weaker entrainment effect in the simulation due to a lack of wind shear.

The temporal evolution of the simulated and observed TKE at several heights is presented in Fig. 7. The TKE reads

\[
TKE(z,t) = \frac{1}{2}(\sigma_u^2(z,t) + \sigma_v^2(z,t) + \sigma_w^2(z,t)),
\]

where \(\sigma_u^2\), \(\sigma_v^2\) and \(\sigma_w^2\) are the variances of the horizontal \(u\), \(v\), and vertical \(w\) wind components. For a better comparison, simulated and observed TKE are estimated using the wind components variances deduced from the integration of the spectra over the wavenumber range of the simulation. By doing this, the TKE associated to large and small eddies observed, but not simulated or resolved in the LES, is removed from the observed TKE. Even with this method, LES underestimates the observed TKE by a factor sometimes as high as 1.5.

In summary, the simulated boundary layer is comparable to the observed one in terms of boundary layer height, wind speed, and dynamical and thermal stability (not shown) near the surface. The lower development of the PBL height of about 200 m and the underestimated TKE by a factor of 1.5 can be partly explained by the directional wind shear which is not simulated. The latter might increase the entrainment and the turbulence dynamical production at the top of the boundary layer. Despite these differences on the main PBL structure, the simulation is realistic enough to evaluate how the turbulence evolves in a convective boundary layer during the AT and the comparison of simulated and observed boundary layer will be analyzed accordingly.

4 Spectral analysis method

A broad overview of the turbulent conditions during the afternoon is depicted through the analysis of the TKE temporal evolution at different heights in the PBL.

The energy distribution among the different eddy scales is then studied through a spectral analysis of the vertical velocity \(w\) within the entire PBL. The evolution of \(w\) spectral characteristics is analyzed by use of an analytical spectral model.

This study focuses on \(w\) because simulated and observed \(w\) spectra are more easily comparable than the spectra of the horizontal components. Indeed, the horizontal components have significant energy at low wavenumber (large scales) in the observations which can not be represented in our simulated domain.

The choice of the analytical spectra is now discussed since several models exist for convective conditions. Among others, the Kaimal et al. (1972) and Kaimal et al. (1976) formulations were established from Kansas experiment observations for the surface layer and from Minnesota experiment observations for the mixed layer. The von Kármán spectral
model (Kärman, 1948) is also widely used for isotropic turbulence. Højstrup (1982) proposed a more generalized model for \( w \) spectra up to \( z/z_i = 0.5 \), based on a stability function from neutral to very unstable conditions. However, many of these analytical models were validated for unstable near surface conditions and most of them are not suitable within the entire convective PBL (Lothon et al., 2009). Among several analytical models tested, the general kinematic spectral model for non-isotropic horizontally homogeneous turbulent field from Kristensen and Lenschow (1989) (named hereafter \( KL89 \)) is the one which best fits the observed spectra at surface and in the boundary layer acquired during the BLLAST field campaign (not shown). For \( w \), the \( KL89 \) model writes:

\[
\frac{S_{K89}(k)}{\sigma^2_w} = \frac{c^o}{2\pi} \frac{l_w}{1 + \frac{2}{\alpha(\mu)} \left( \frac{\Lambda_k}{\sigma_w} \right)^{2\mu} + \left( \frac{\Lambda_k}{\sigma_w} \right)^{5/3(\mu+1)}},
\]

where

\[
\alpha(\mu) = \pi \frac{\mu \Gamma\left( \frac{2}{\alpha(\mu)} \right)}{\Gamma\left( \frac{1}{\alpha(\mu)} \right)}
\]

\( k \) being the wavenumber along the trajectory of the airplane, or along the west-east axis in the simulation (which is also the mean wind direction in the simulation), and in the mean wind direction for surface measurements. \( \Gamma \) is the gamma function. \( c^o \) is a coefficient which adjusts the amount of energy because \( \sigma^2_w \) is calculated over a limited range of wavenumbers. This model has two other characteristic parameters: the integral length scale \( l_w \), which is a characteristic scale corresponding to the scales over which \( w \) remains correlated with itself (Lenschow and Stankov, 1986), and a sharpness parameter \( \mu \), which governs the curvature of the spectra in the region of the peak, between the low wavenumber range and the inertial subrange. The larger \( \mu \), the sharper the peak. According to Eq. 2, the \( KL89 \) model gives the Kaimal et al. (1972) spectrum for \( \mu = 0.5 \) and the Kärman (1948) spectrum for \( \mu = 1 \). It is thus a more generalized model, able to adapt to a larger range of conditions. Note that \( l_w \) is related to the wavelength of the energy density maximum (\( \Lambda_w \)) by a monotonic function of \( \mu \):

\[
\Lambda_w = \left\{ \frac{5}{3} \sqrt{\frac{\mu^2 + 6}{5} \mu + 1} - \left( \frac{5}{3} \mu + 1 \right) \right\} ^{\frac{1}{2}} \frac{2\pi}{\alpha(\mu)} l_w.
\]

This model is fit to each observed and LES spectrum, by finding the best \([c^o, l_w, \mu] \) triplet using a logarithmic least squares difference method.

The integral scale of \( w \) is usually defined from \( w \) autocorrelation function \( R_w \) as:

\[
L_w = \int_0^\infty R_w(r)dr,
\]
0.6 - 0.75z_i slice-averaged). This figure shows first, the ability of the simulation to properly reproduce both the energy production domain and the inertial subrange, and second, the ability of the analytical spectral model to fit well the observed and simulated spectra in mid-afternoon convective conditions (1500 UTC) and at the end of the afternoon (1800 UTC).

For those two examples, IQ_{OBS} = 0.11 and IQ_{LES} = 0.02 at 1500 UTC, and IQ_{OBS} = 0.10 and IQ_{LES} = 0.015 at 1800 UTC. In general, the quality index for the observations are about 5 to 10 times larger than for the LES (not shown). This is due to the lack of statistics at large scales in observations, leading to larger fluctuations in the spectral density energy for the first domain (low wavenumbers), whereas the LES spectra are averaged along the north-south direction, reducing the variability.

We also found that the quality index for observed and simulated data generally remained constant until 1900 UTC, except a slight increase of IQ_{LES} for data above 0.6 z_i after 1830 UTC. This means that the spectra fit is equally reliable throughout the AT, allowing the study of the time evolution of the spectra characteristics from the convective conditions until near neutral conditions. This result should be highlighted in the case of simulated spectra given the overly dissipative nature of the subgrid-scale models in the LES (Meneveau and Katz, 2000).

The spectra changes throughout the AT are already noticeable in Fig. 8: \Lambda_{w} shifts toward smaller wavelength, \Lambda_{w} increases, the spectra flatten and the inertial subrange slope changes. This is further quantified and discussed in the following section.

5 Results

5.1 TKE decay within the entire PBL

Most previous studies investigated either vertically integrated simulated TKE over PBL depth, or measured TKE in the surface layer. The TKE decay according to height remains sparsely documented (Grant, 1997; Goulart et al., 2010).

Figure 9a shows the evolution of half-hour averaged hourly vertical profile of simulated TKE from 1130 UTC to 1830 UTC. The profiles show that TKE decreases within the whole depth of the PBL, but that there is a one-hour delay between the start of the decay at the top and the start at the bottom: at 1230 UTC, the TKE continues to increase in the lower PBL, while it has started to decrease in the upper part. After 1530 UTC, the decay is homogeneous over the vertical. This differential TKE decay will be named TKE top-down decay hereafter. This result is consistent with Grimsdell and Angevine (2002) and Lothon et al. (2014) studies which revealed, with remote sensing observations, a decay of TKE dissipation rates from top to bottom. Shaw and Barnard (2002) also studied the decay with Direct Numerical Simulation (DNS), based on a realistic surface flux decay. They found that the turbulence is maintained at the surface relative to upper layers, which they explain with shear at surface.

In this study, the simulation shows this top-down evolution likely because the shear in wind direction at the top of the boundary layer is weak and does not maintain the dynamical turbulence production. We can expect a reduced top-down effect in the reality since there is shear in direction which is not simulated.

Turbulence anisotropy (see Fig. 9b), considered here as the ratio of the horizontal to the vertical wind variances, gives highlights on the turbulence structure evolution during the TKE decay. Before 1630 UTC, turbulence anisotropy remains larger than 1 in the mid-PBL, which is in agreement with the dominant vertical motion of the convective eddies. In the upper and lower parts of the PBL, turbulence anisotropy is larger than 1, due to small vertical velocity variance close to the surface and the entrainment zone (so called ‘squashed’ turbulence (Lothon et al., 2006)). The anisotropy ratio becomes larger than 1 only after 1730 UTC in the middle of the PBL, but increases close to the top as early as 1230 UTC. The change in anisotropy, like the TKE, starts early in the upper PBL, with an increasing momentum transfer from vertical to horizontal components during the decay process.

5.2 Spectral analysis

5.2.1 Evolution of the vertical velocity’s spectral slopes

The slopes of the simulated and observed spectra are first analyzed because (1) they are key characteristics of the turbulence spectra and, (2) the KL89 spectral model assumes for kS(k) the theoretical slope of 1 and \(-2/3\) for low and high wavenumber range, respectively. The slopes are estimated by linear regression on kS(k) for the wavenumber first and third ranges defined in Section 4.

In the low wavenumber range, the slopes of the simulated and near-surface observed spectra are close to the theoretical value of 1 and remain approximately constant during the whole day (see Fig. 10a). The spectral slopes of airborne measurements are steeper than the theory predicts and vary from 1.5 to 2.5. This result illustrates the weak statistical representativity of large scales along aircraft flight leading to scattered spectra slope estimates in this wavenumber range.

In the inertial subrange, both simulated and aircraft data reveal steeper slopes than the theoretical value of -2/3, even during the fully convective period (Fig. 10b). Steeper inertial subrange slopes were previously observed with vertically pointing ground based lidar (Lothon et al., 2009) and with airborne high frequency in situ measurements (Lothon et al., 2007). The theoretical -2/3 slope is based on the hypothesis of isotropic turbulence. Therefore, a possible explanation for these steeper slopes in convective
conditions could be the loss of isotropy in real conditions and in particular the role of convective structures and the associated anisotropy. As mentioned before, in section 5.1, they are responsible for anisotropy smaller than one. We believe that the more ‘coherent’ or organized the $\mu$ field, the smaller the anisotropy and the steeper the slope. But this explanation needs further work for confirmation.

At the end of the afternoon, the slopes consistently flatten in both LES and aircraft data. This flattening appears to behave differently according to height in two ways: (1) it occurs earlier at the top of the PBL (around 1600 UTC) than in the lower layers (after 1745 UTC at 0.15$z_i$), (2) the lower in the PBL, the smaller the flattening. These delayed and reduced changes with decreasing altitude are consistent with the constant - 2/3 slope during the whole day near the surface.

5.2.2 Characteristic length scales

The integral scale is one of the two spectral characteristics determined from the fit of the $KL89$ analytical spectral model.

We verified that these integral scale estimates ($l_w$) were similar to estimates of integral scales ($l_w$) based on the autocorrelation function (Eq. 5) which is more generally used. The two methods were found to be consistent with each other and to give similar temporal evolution of integral scale (not shown). Hereafter, only $l_w$ is considered.

The temporal evolution of $l_w$ obtained with aircraft and surface data and with the simulation at different heights, is presented in Fig. 11. At midday, the length scales verify what is found in literature, with a value around 200 m (about 0.2$z_i$) in the middle of the mixed layer (Lenschow and Stankov, 1986) with aircraft observations and Dosio et al. (2005) with LES, among others. Smaller length scales are observed and simulated at the top and at the bottom of the mixed layer because of 'squashed' eddies near the interfaces. $l_w$ remains approximately constant until 1700 UTC, and then increases above 0.15$z_i$ for both LES and aircraft data. The higher the considered level, the sharper the $l_w$ increase.

Close to surface, $l_w$ remains constant until 1700 UTC at a value of 10 m, then decreases to 5 m. As expected, the 60 m mast data provide longer $l_w$ than at the surface, but with a large scatter (between 30 and 80 m) making difficult the estimate of $l_w$ tendency with time at that height.

5.2.3 Shape of the spectra

The spectral shape is depicted by the $\mu$ sharpness parameter (Eq. 2). Figure 12 shows the temporal evolution of $\mu$ that gives the best fit of the spectra for simulation, aircraft and surface data. Above 0.15$z_i$, $\mu$ remains constant at a value of about 2 until 1600 UTC, aircraft and simulated data giving similar results. Those results are similar to those found by Lothon et al. (2009) with ground-based lidar, who also observed sharper spectra than Kaimal spectra ($\mu = 0.5$) in the middle of the PBL. After 1600 UTC, $\mu$ decreases, meaning that the turbulence spectra flatten during the late afternoon transition associated with a broadening of the energy containing wavenumber range above 0.15$z_i$. This seems consistent with the theoretical spectral analysis by Goullart et al. (2010) (see their Fig. 6 bottom in convective boundary layer). On the contrary, close to surface and at 60 m height, $\mu \approx 0.5$ throughout the day, which corresponds to the spectral model from Kaimal et al. (1972) and means that the energy wavenumber range remains large during the LAT. In $KL89$ analytical model, $\mu$, $l_w$ and $\Lambda_w$ are linked by Eq. 4 which gives higher $\Lambda_w/l_w$ for higher $\mu$ (Lenschow and Stankov, 1986). As noticed in Fig. 8, $\Lambda_w$ drifts slightly toward smaller eddies. Keeping in mind that $\Lambda_w$ represents the distance between two structures and $l_w$ represents the width of a structure, this means that during the LAT, the thermals become closer from each other whereas the increase of $l_w$ means the thermals become larger. This is consistent with a decreasing skewness of $w$ as time evolves, which we do find in both observation and LES (not shown).

5.3 Timing of the changes

The previous results illustrate the changes of turbulence characteristics throughout the afternoon according to height. The times when these characteristics start to change are now quantified using the simulation data above 0.15$z_i$, the tower measurements at 60 m and the near surface moor and corn data. The time of change for a parameter $x$ is noted $t_x$ (Fig. 13). For $\mu$, $l_w$ and the slope, it is the time when the decay rates of these spectra parameters depart from their mean value by more than three times their standard deviation (the decay rates are estimated over 1.5 h and their means and standard deviations are calculated between noon and 1400 UTC). Because of the diurnal cycle of the TKE and the horizontal and vertical velocity variances, this method could not be applied to determine the time change of these parameters. $t_{TKE}$, $t_{u'^2}>$ and $t_{u'^2}+$ were thus the time when the decaying rate of the parameter (estimated by linear regression over 1.5 h) becomes larger than an arbitrary threshold of -0.02 m$^2$s$^{-3}$.

As already noticed in section 5.1, the TKE first decreases at the top of the boundary layer half an hour after the start of the AT (Fig. 13). That is, once the surface flux starts to decrease, the surface-driven turbulence does not rise up to the top of the CBL anymore. This induces that turbulence decreases first at the top of the PBL whereas it is maintained longer under 0.15$z_i$. The TKE decrease is exclusively driven by the vertical velocity variance, which decreases at the top of the PBL one and half hour before the maximum of the surface buoyancy flux. The early decrease of the vertical velocity variance is counter-balanced in TKE by the delayed change of the horizontal wind variance. This
implies an increase in the anisotropy of the velocity variances in the early stage of surface flux decrease.

The change in other spectral parameters (length scale, sharpness and slope) is observed much later, during the last two hours before the zero surface buoyancy flux. The vertical profiles of $t_{lw}$, $t_{slope}$, and $t_{\mu}$, indicate an increase of integral scales, a flattening of the inertial subrange slope and a flattening of the spectra, appearing first at the top of the boundary layer and rapidly reaching the lower layers.

Near the surface and at 60 m, a very weak evolution of the spectra is observed. The spectra keep the same sharpness, similar to Kaimal spectra, with a constant slope of $-2/3$ in the inertial subrange, and a very slightly decreasing $l_{lw}$. These results are in continuity with the spectra behavior above 0.15 $z_i$. Indeed, $\mu$ decreases from around 2 in convective conditions to 0.5 at the end of the AT in the whole upper layer and the $l_{lw}$ increase in the upper layers is less and less pronounced with decreasing height.

5.4 Discussion

The above analysis of the evolution of the turbulence structure during the AT suggests us to separate this period in two stages: early and late afternoon.

In the early afternoon, from the occurrence of the buoyancy maximum until about two hours before sunset, (1) the TKE decreases within the whole PBL, with a one-hour delay between the upper part (earlier decay) and the lower part of the PBL (postponed decay), (2) the vertical profile of anisotropy does not change much within the PBL, except close to the top, and (3) the spectra maintain the characteristics of the fully-developed convective boundary layer, with similar integral scales and sharpness parameter.

In the late afternoon, from two hours before sunset until when the surface buoyancy flux reduces to zero, (1) the TKE decreases more rapidly than during the early AT within the whole PBL, (2) turbulence anisotropy increases abruptly within the PBL, starting initially near the PBL top, and (3) the shape of the spectra evolves, with a decrease of the sharpness parameter, a flattening of the inertial subrange slope, an increase of the integral length scales in the mid and upper PBL. The higher in the PBL, the stronger the increase of the integral scales, with very slight changes of the spectra shape observed close to the surface.

The two stages of the TKE decay found in this study remain consistent with previous results found by Nadeau et al. (2011) and Rizza et al. (2013a). Both authors showed a decrease of the TKE following a $t^{-n}$ power law with a continuous increase of $n$. Nadeau et al. (2011) defined two main stages characterized by $n$ around 2 and 6 respectively. Rizza et al. (2013a) added a preliminary stage with $n$ equal to 1. Our first stage includes $t^{-1}$ and $t^{-2}$ power laws, and the second one includes $t^{-6}$. However, it seems somehow arbitrary to characterize our two stages by a specific value of $n$ since it evolves continuously. This study focuses on the link between the structure of the turbulence and the TKE evolution. Also, the TKE budget evolution in time was of any help to explain the two stages of the TKE decrease. Whilst the different terms do decrease with time, their respective contribution to the TKE tendency hardly changes from the first to the second stages (not shown).

Our understanding of the two different stages of the AT is that during the early afternoon, the buoyancy flux remains large and its decay is slow enough, to give time to the PBL to adjust to the change and to remain in quasi-steady balance. In other words, the convective time scale $t_\ast$ is small enough ($\sim 9 \text{ min}$) relative to $\tau_f$ ($\sim 5.8 \text{ h}$), to allow this quasi-steady state. The spectral characteristics remain similar to what they are at maximum surface buoyancy flux. Buoyancy remains a dominant influence during this stage, which leaves predominance to the vertical velocity variance and convective structures. The latter, with a characteristic horizontal length typically linked to the PBL depth, could maintain a sharp spectral peak. Predominance of convective structures might also be at the origin of the steep inertial subrange slope.

Close to surface, where these convective structures are not yet well shaped, inertial subrange slope is $-2/3$.

On the contrary, during the late afternoon, $t_\ast$ increases (about 20 min at 1700 UTC) and the buoyancy flux gets too small for the PBL to maintain the vertical consistency of the turbulence structure from surface up to the top of the PBL. The impact of surface buoyancy decreases faster than that of entrainment during this period: although the entrainment flux magnitude diminishes, entrainment occurs over a broader vertical depth extending down to 0.6$z_i$ (Fig. 5).

An increase of the entrainment role could explain the increase of the vertical velocity integral scales (Lohou et al. (2010) and Canut et al. (2010)) which is observed in the upper PBL during the late afternoon during our BLLAST case. The vertical velocity integral scales increase is consistent with the results of Sorbjan (1997) but differs from those of Pino et al. (2006). This could be due to the progressive cease of the surface flux in Sorbjan (1997) and Grant (1997), versus the sudden shut-off in Pino et al. (2006). In the surface layer, the decrease of the integral scales is consistent with the observations made by Grant (1997) and with the results of Kaimal et al. (1972).

The flattening observed in the inertial subrange during the late afternoon is difficult to explain because one could expect a steeper slope in inertial subrange when the flow becomes less turbulent, assuming that the smaller scales will dissipate faster than the larger scales. However, hypotheses could be made to explain the observed flattening of the spectra in inertial subrange: (1) the increase of anisotropy might be associated with such change of the cascade, (2) if the turbulence is now freely decaying, without influence of coherent structures and vertical velocity dominancy, the cascade could become more efficient, resulting in flattening slope according to Moeng and Wyngaard (1988). In any case, it seems that
with the turbulence being no longer fully forced, the criteria for locally isotropic turbulence are no longer met. The theoretical model of TKE spectrum proposed by Goulart et al. (2010) could be an interesting tool to further understand this slope change since it considers anisotropy of turbulence through the $KL_{89}$ analytical spectrum, but also into some of the terms of the TKE budget which might impact on the inertial subrange slope.

The progressive shut-off of the surface heat fluxes is shown to be an important aspect of the AT. Nieuwstadt and Brost (1986) and Pino et al. (2006) who analyzed simulations with a sudden shut-off of the buoyancy flux pointed out what they called a demixing process which infers a negative buoyancy flux within the whole PBL. The impact of entrainment in that case might be overestimated. Similar to Sorbjan (1997), when progressively transitioning through the afternoon from surface buoyancy dominated to entrainment dominated regime, the demixing process is strongly reduced and limited to the half-upper part of the PBL.

One might wonder whether these results could be impacted by the initial conditions. The use of all the airborne measurements acquired during the BLLAST experiment shows the general trend of an increasing integral scale during the late afternoon (not shown). However, it would be useful to complete this study with some additional simulations either targeting other BLLAST IOPs or performing some sensitivity analyses. Wind shear could be particularly under focus as Nieuwstadt and Brost (1986), Pino et al. (2006) or Goulart et al. (2010) found that strong wind shear at the top and bottom of the PBL delays the decay.

6 Conclusions

This study is based on the use of analytical spectra to depict and quantify changes in the vertical velocity spectra throughout the AT and according to height. BLLAST aircraft and surface station measurements are used to study the turbulence spectral evolution on 20 June 2011. A Large-Eddy Simulation constrained by observed conditions during BLLAST, but significantly simplified, allows us to investigate a continuous spectra analysis in time and height.

The simulated data, even with simplified forcings and initial conditions, are in a satisfactory agreement with the airborne, radiosonde and surface observations. The model reasonably simulates the turbulence structure through the afternoon with a resolution and a domain size allowing a good fit of the simulated spectra with the Kristensen and Lenschow (1989) analytical model above 0.15 $z_i$.

Two main conclusions can be drawn from this study, giving essential highlights on the turbulence evolution in time and height:

(1) This study shows for the first time the different steps occurring during the AT, which is defined as the period starting at the maximum surface buoyancy flux and ending when the buoyancy flux reaches zero. The early afternoon (first phase from 0 to 0.75$\tau_f$) is characterized by a low-rate decrease of the energy level, but the turbulence characteristics remain similar to those during fully convective conditions: similar turbulence length scales and cascade characteristics from large to small eddies. During the late afternoon (second phase from 0.75 to 1$\tau_f$), TKE decay rates increase and turbulence characteristics evolve rapidly implying very different eddy size and energy transfer.

(2) The second important point concerns the turbulence evolution along the vertical. The changes observed either on TKE decay (during the early afternoon) or on $w$ spectral shape (during the late afternoon) start at the top of the boundary layer. Furthermore, the higher within the PBL, the stronger the spectra shape changes. These results show that the top of the boundary layer is first affected by the changes.

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Fig. 2. Observed vertical profiles of (a) the potential temperature $\theta$ and (b) the wind direction on the 20 June 2011. The black dashed lines represent the initial profiles of the LES.

Fig. 3. Temporal evolution of (a) surface sensible ($H$) and (b) latent ($LE$) heat fluxes over several vegetation coverages, on 20 June 2011. Dashed black curves stand for the surface flux used as boundary conditions for the LES. The vertical dashed lines stand for the times of maximum surface buoyancy flux (at 1200 UTC) and zero value (at 1750 UTC).
Fig. 4. Vertical profiles of (a) $\theta$, (b) $r$, (c) wind speed (WS), (d) wind direction (WD) observed (solid lines and dotted lines for WD) and obtained by LES (dashed lines).

Fig. 5. Vertical profiles of the buoyancy flux normalized by the surface buoyancy flux at 1200 UTC according to the normalized height $z/z_i$.

Fig. 6. Temporal evolution of $z_i$ in the simulation (black), observed by the UHF wind profiler (blue) and depicted using radiosondes (RS) measurements (red dots).
Fig. 7. Temporal evolution of the resolved TKE (subscript RES) at different heights in the simulation (different colors). TKE deduced from aircraft and surface (subscript OBS) spectra integrated over the LES spectra wavenumber range (open and filled circles, respectively). The vertical dashed lines stand for the times of maximum surface buoyancy flux (at 1200 UTC) and its zero value (at 1750 UTC).

Fig. 8. Normalized $w$ spectra at (a) 1500 and (b) 1800 UTC from both aircraft (black) and LES (grey), fitted with the $KL89$ analytical spectral model (thick lines). The vertical continuous line represents $\Lambda_w$, the maximum energy wavenumber and the dashed vertical lines represent $k_1$ and $k_2$, the limits of the low wavenumber range and of the inertial subrange, defined as $k_1 = \pi/\Lambda_w$ and $k_2 = 4\pi/\Lambda_w$. 

Fig. 9. Vertical profiles of the total (resolved and subgrid (subscript TOT)) (a) TKE and (b) anisotropy at several hours during the AT in the LES.

Fig. 10. Temporal evolution of the slopes in (a) the low wavenumber range and (b) the inertial subrange of the $w$ spectra obtained by LES (continuous lines), aircraft and surface measurements (open and filled circles) at different heights (colors). The horizontal black lines stand for the theoretical expected values.
Fig. 11. Temporal evolution of $l_w$ calculated from the $KL89$ analytical model fit on LES (continuous lines), aircraft (open circles) and surface (closed circles) spectra at different heights (different colors). Note that $l_w$ at surface and at 60 m are multiplied by a factor 10. The vertical dashed lines stand for the times of maximum surface buoyancy flux (at 1200 UTC) and its zero value (at 1750 UTC).

Fig. 12. Temporal evolution of the parameter $\mu$, obtained from the $KL89$ analytical model, by using LES (continuous lines), aircraft (open circles) and surface (closed circles) data. The vertical dashed lines stand for the times of maximum surface buoyancy flux (at 1200 UTC) and its zero value (at 1750 UTC).

Fig. 13. Vertical profiles of the timings of changes observed in the evolution of the TKE, the vertical and horizontal variances, $l_v$, $\mu$ and the inertial subrange slope of $w$ spectra. $t'$ is defined as the time when $H$ is maximum (i.e at 1200 UTC).