J9.1 ROLE OF THE BOUNDARY LAYER PROCESSES IN UNDERSTANDING THE CO_2-BUDGET

David Pino *
Applied Physics Department, Technical University of Catalonia, and Institute for Space Studies of Catalonia (IEEC), Barcelona, Spain
Jordi Vilà-Guerau de Arellano
Meteorology and Air Quality Section, Wageningen University, Wageningen, The Netherlands

1. INTRODUCTION

Boundary layer dynamics, including surface processes determine the daily evolution of temperature and moisture in the atmospheric boundary layer (ABL, Lemone *et al.*, 2002). Moreover, turbulent mixing drives the exchange of CO_2 between the atmosphere and biosphere and, finally, the advection influences the distribution of carbon dioxide near the surface (Yi *et al.*, 2000; Werner *et al.*, 2006; Eugster and Siegrist, 2000), and as a consequence Net Ecosystem-atmosphere Exchange (NEE) of carbon dioxide.

NEE is continuously estimated around the world usually from measurements at one height near the ground of the time evolution of the CO_2 concentration and turbulent flux (Valentini *et al.*, 2000; Baldocchi *et al.*, 2001). In these observations, among other approximations, advection is supposed negligible (Yi *et al.*, 2000), and a well-mixed boundary layer is considered during the whole day.

In this study the diurnal variability of the CO_2 concentration is studied by means of tower measurements, mixed-layer theory and Large-Eddy simulations done with the Dutch model DALES (Heuss *et al.*, 2010). The work presented here is an extension of Casso-Torralba *et al.* (2008), where observations were presented. Particular attention is devoted to analyze the role of boundary layer processes on the CO_2 evolution and to study the uncertainties in the calculation the Net ecosystem-atmosphere Exchange for CO_2.

2. OBSERVATIONS

At the Cabauw site, located in the center of The Netherlands, meteorological and fluxes measurements are taken continuously. The site lies in an open field nearly completely covered by short grass which extends for several hundreds of squared meters (see Beljars and Bosveld (1997) for detailed description of the site). In this site, vertical profiles of wind, temperature, humidity and carbon dioxide are measured along a 213 m meteorological tower. Measurements for temperature are taken at 2, 10, 20, 40, 80, 140, and 200 m, whereas CO_2 concentration is recorded at 20, 60, 120, and 200 m. Carbon dioxide observations have been previously described by Werner *et al.* (2006).

Fluxes of momentum, sensible and latent heat and carbon dioxide are also measured at 10 Hz at 5, 60, 100, and 180 m height. For further description on flux measurements, see Bosveld *et al.* (2004) and Werner *et al.* (2006).

2.1 *Selected day*

A convective day with well mixed boundary layer has been selected to study simultaneously the temporal evolution of the carbon dioxide concentration, and virtual potential temperature.

25 September 2003 (Casso-Torralba *et al.*, 2008) was a convective day with negligible large scale advection and few clouds observed. The nearly sinusoidal pattern in time of the measured short wave downward radiation confirms the presence of clear skies. Measurements from the radiosonde performed at De Bilt at 12 UTC indicate a well mixed layer of about 1200 m for that day, which is in agreement with what is found by analyzing wind profiler measurements. Constant 4-5 m s^{-1} winds regardless of height are measured during the day.

3. NUMERICAL SETUP

To further understand the evolution of the convective boundary layer (CBL) and to study the importance of the boundary layer processes on CO_2 concentration, a mixed-layer model (Vilà-Guerau de Arellano *et al.*, 2004 and Pino *et al.*, 2006) and the dutch Large-Eddy simulation model (DALES; Heus *et al.*, 2010) have been used.

The same initial conditions have been considered for both models based on observations. Moreover, both models include the same time evolution of the surface fluxes (sensible, latent and carbon dioxide) based on observations.

Table 1 summarizes the initial and surface values for the virtual potential temperature, specific humidity and the carbon dioxide prescribed in the mixed layer model and DALES runs for the selected day. As figure 1 shows, the prescribed surface fluxes follow a sinusoidal function to account for the evolution over time.

Large-Eddy Simulation domain has 12.6×12.6×3 km^3 with grid spacing $\Delta x = \Delta y =$ 50 m and $\Delta z =$ 12 m. The total simulation time was 10 hours, and the slab horizontal averaged model output was recorded every five minutes. The final statistics used in this work were obtained by performing a temporal averaging every 30 minutes. DALES bulk results for θ_v and CO_2 concentration are calculated by averaging the vertical profile from the surface up to the boundary layer depth.

* *Corresponding author address:* David Pino, Applied Physics Department, Technical University of Catalonia, Esteve Terrades 3, 08860 Castelldefels, Spain; e-mail: david.pino@upc.edu

	25/09/2003(6 UTC)
	MXL/DALES
z_i (m)	120
δ (m)	0/24
$\overline{\theta}$ (K)	284
$\Delta\theta$ (K)	4
β	0.2+5($u_*/w_*)^3$/-
γ_θ (K km^{-1})	3.6
$\overline{q}$ (g kg^{-1})	4.3
Δq (g kg^{-1})	-0.8
γ_q (g kg^{-1} km^{-1})	-1.5
$\overline{CO_2}$ (ppm)	410
Δ CO_2 (ppm)	-22
γ_{CO_2} (ppm km^{-1})	-30

Table 1: Initial and prescribed values used for the main boundary layer variables for the mixed layer model and DALES based on the observations taken at Cabauw on 25th September 2003. Notice that β is explicitly calculated in the DALES.

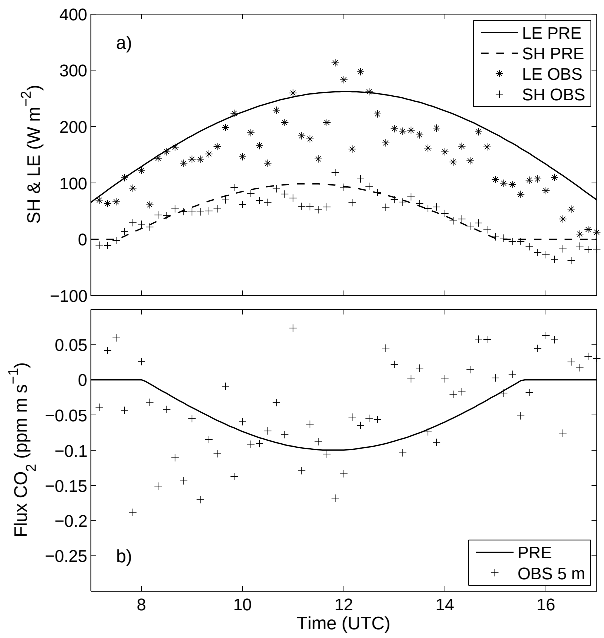

FIGURE 1: Observed (OBS, symbol) evolution of the surface (a) heat fluxes, and (b) carbon dioxide flux on 25th September 2003. The lines represent the prescribed fluxes (PRE) in the simulations.

4. RESULTS

4.1 *Evolution of the mean variables*

As figure 2 shows, both MXL and DALES results fit well for the studied day the observed diurnal evolution of the mixed-layer depth, virtual potential temperature, and carbon dioxide concentration. The main characteristics of the comparison can be summarized as follows:

- Both models reproduce satisfactorily the mixed layer depth observations, except at the middle of the day when scattered clouds were observed above the site, and the measurements of the boundary layer depth by the wind profiler can be affected by them. This fact can be observed in figure 2a by the small jump that appeared. As can be observed, differences between z_i, (defined as the height of the minimum buoyancy flux) and h_1 (defined as the height of the maximum virtual potential temperature gradient) obtained by DALES were observed, being always $h_1 > z_i$. As expected, z_i evolution is similar to MXL calculations. Both underestimate observational values. However, h_1 fits better the observations.

- The observed diurnal evolution of temperature and carbon dioxide at different tower levels and simulated with MXL and DALES for the 25 September 2003 is shown in figures 2b. c. A total increase of about 9 K is observed for the potential temperature from 7 to 16 UTC and measurements of carbon dioxide mixing ratio at 5 m show an important decrease of 50 ppm during the same period of time. The morning transition from a stable boundary layer to an unstable mixed layer occurs between 7 and 8 UTC. The dramatic decrease of 30 ppm of the CO_2 mixing ratio at 5 m between 7 and 9 UTC indicates the mixing of entrained air with low content of CO_2 and the uptake by plants. The vertical gradients of potential temperature and carbon dioxide mixing ratio tend rapidly to zero in the upper levels during this morning transition until both scalars reach a constant value with height once the height of the growing mixed layer reaches the level of 200 m at 9 UTC. The strong diurnal variability of both scalars has a clear maximum for the potential temperature of 291 K at around 16 UTC. Similarly, a minimum of 375 ppm for the CO_2 mixing ratio occurs earlier at 14 UTC. This strong variability of the CO_2 mixing ratio during the transition from a stable boundary layer to an unstable mixed layer is also observed by Yi *et al.* (2000) and Werner *et al.* (2006a). The general observed features of the evolution of θ and CO_2 concentration were well simulated with the MXL and the DALES models.

  An interesting observed feature of the transition period is that temperature reaches a constant value with height at 9 UTC whereas CO_2 is not well mixed until 10 UTC. This is due to the slow vegetation uptake which yields to this delay in the vertical homogenization of CO_2 (see Casso-Torralba *et al.*, 2008).

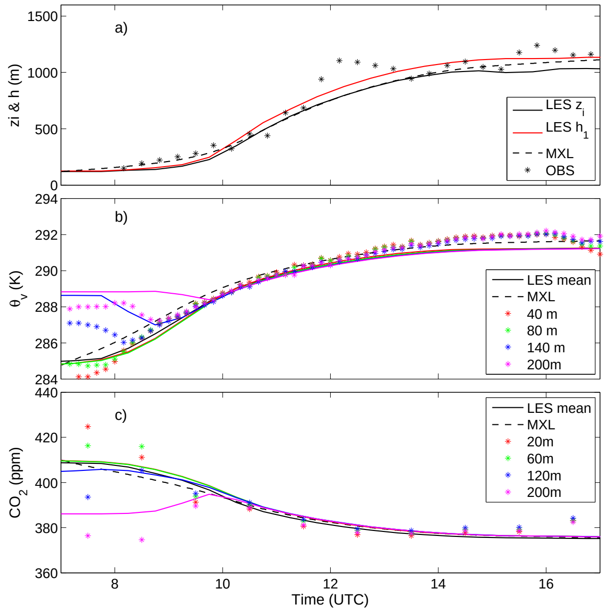

FIGURE 2: Observed (asterisks) and simulated by means of DALES (solid lines) and by means of MXL (dashed line) diurnal evolution during 25th September 2003 of (a) the boundary layer depth, (b) virtual potential temperature and (c) CO_2 concentration. In a) z_i and h_1 are the height of the minimum buoyancy flux and of the maximum virtual potential temperature gradient, respectively. The DALES results at the measurement heights and its mean value in the mixed layer are shown in b) and c).

However, DALES produces a well mixed boundary layer for both variables around 10 UTC.

4.2 *Heat and carbon dioxide budget*

Casso-Torralba *et al.* (2008) observed heat and carbon dioxide fluxes varying linearly with height during the studied day. They found values of the ratio between entrainment to surface fluxes $\beta > 0.4$ and $\beta_c \approx$ 3-5 for heat and carbon dioxide respectively.

The values obtained with DALES and MXL follows the typical diurnal evolution with large entrainment ratios during the morning and during the afternoon (not shown). Most of the day due to the low winds prescribed $\beta < 0.2$. Moreover, the MXL model, in order to reproduce the observations, has to use a larger value of β (see Pino *et al.*, 2006). During the whole simulation $\beta_c > 1$, which means that the concentration of CO_2 is characterized by a dominance of the dilution processes due to the entrainment of free tropospheric air masses with low CO_2 concentrations.

Once we have shown that the simulations reproduce quite reasonable the observations this section is devoted to analyze the importance of advection and flux divergence in the evolution of two scalars: temperature and CO_2 concentration. In convective situations like the one present here, the horizontal flux divergence in the horizontal direction is expected to be smaller than the vertical turbulent flux divergence (Davies, 1992; Yi *et al.*, 2001). Therefore, the conservation equation of any scalar quantity, if molecular diffusion and subsidence are also neglected, reads:

$$\frac{\partial \bar{c}}{\partial t} + \bar{u}\frac{\partial \bar{c}}{\partial x} + \bar{v}\frac{\partial \bar{c}}{\partial y} + \frac{\partial \overline{w'c'}}{\partial z} \approx \overline{s_c}, \qquad (1)$$

where the overline represents Reynolds averages, $\overline{w'c'}$ is the turbulent vertical flux of the scalar and $\overline{s_c}$ includes the sources and sinks of the scalar. This equation includes the tendency/storage term (TE, first term of the left hand side), the contribution of horizontal advection (A, second and third terms) and the last left hand side term is the vertical divergence of the flux (DF), which describes the contribution of the vertical exchange of the scalar quantity in the scalar conservation equation due to the vertical turbulent flux.

Under clear convective conditions, (as the presented here) buoyancy is the main mechanism driving turbulence. In this situation, conserved variables are almost constant except in the surface layer. Therefore, it can be demonstrated (Stull 1988), that in this quasi-steady condition, fluxes of this conserved variables are linear with height. This is exactly one of the assumptions of the MXL model. Casso-Torralba *et al.* (2008) already showed the linearity of the vertical profiles of the observed heat and CO_2 fluxes in the middle of the day. Consequently, the DF term is retrieved from the linear fitting of the observed fluxes. Their calculations showed that the deviation of the measured fluxes from the linear trend ranges between 10 to 30 % during the daytime hours both for heat and CO_2. In the first morning hours this deviation can be as high as 50-60 % due to the transition from the nocturnal stable regime to unstable conditions during the day.

For the MXL model the DF is exactly the slope of the profile. Finally, to extract the flux divergence from the DALES results, the same heights of the tower measurements were used. If the source and sink term, s_c, is included in the DF term, advection can be calculated as the residual of equation (1). Figure 3 shows the time evolution of the DF and TE terms of budget of (a) heat and (b) CO_2 concentration.

Several conclusions can be listed from this figure:

- The minimum in the storage term of the CO_2 flux is due to the export of CO_2 stored during the night in the nocturnal boundary layer.

- It can be observed in figure 3 that the storage and the divergence of the flux terms have similar values but of opposite sign. As a consequence, the temporal variability of θ and CO_2 is mainly dependent on the surface fluxes and the exchange flux at the entrainment zone. The divergence of the flux is estimated to be about 80-90% of the storage term, whereas advection represents only 10-20% of the time evolution

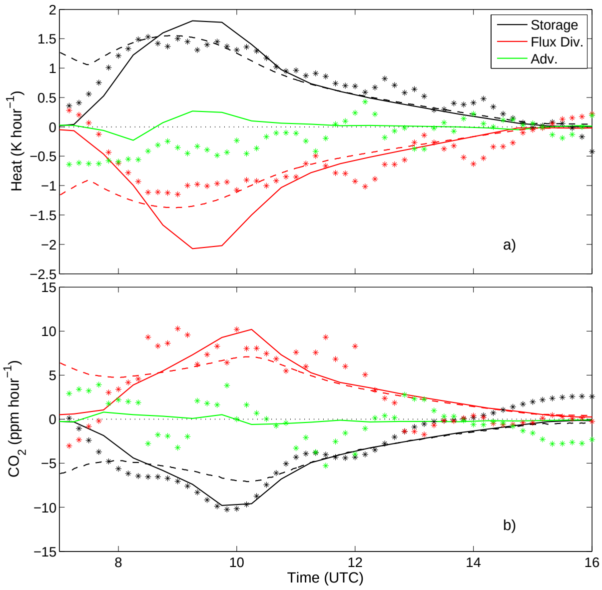

FIGURE 3: Evolution during 25th September 2003 of the different terms (tendency: black, flux divergence: red, advection: green) of the (a) heat and (b) CO_2 budgets calculated by using the observations (*), and obtained by the DALES (solid lines) and the mixed-layer model (dashed lines). The advection term is calculated as a residual.

of both scalars. Results are in accordance with previous analysis of that day (Bosveld *et al.*, 2004) where the advection of heat was found to be small. The estimation of the advection term was done by using the Regional Atmospheric Climate Model (RACMO) of KNMI run in forecast mode. The model in this previous study shows values of warm advection of about 0.15 K h^{-1}, which compares well with the observed values. Notice that our sign convention is that negative advection represents advected warm air. Notice that surface fluxes can be slightly underestimated due to eddy-covariance systematic errors. If so, the contribution of the divergence of the flux would be even larger and thus the estimated advection would be in closer agreement with the model. The end of the growth of the convective boundary layer is reflected in Figure 9 at around 14-15 UTC, causing a negligible change on time of the scalars (no storage) and constant fluxes with height (no divergence of the flux), which gives place to the maximum for θ and minimum for CO_2 shown in figure 2.

- DALES and MXL results fit the observed values for the heat and CO_2 budget. As it was expected, during the morning and the afternoon simulated profiles weren't linear, sensible heat fluxes were negative (prescribed as zero, see figure 1) and the models weren't able to reproduce the observations.

5. NET ECOSYSTEM-ATMOSPHERE EXCHANGE CALCULATIONS

5.1 *Influence of advection and well-mixed boundary layer*

By using 3D sonic anemometers, in order to infer the Net Ecosystem-atmosphere Exchange (NEE), CO_2 fluxes are continuously measured in several automatic stations placed in different land-use characteristics, around the world (see for instance the FLUXNET project in http://www.fluxnet.ornl.gov/fluxnet/index.cfm and Baldocchi *et al.*, 2001). To calculate NEE from observed fluxes and concentrations equation (1) have to be integrated over a control volume which height goes from the surface to the measurement height (z_m) and having an horizontal dimension close to the tower footprint. NEE, is by definition:

$$NEE = \int_0^{z_m} \overline{s_c} dz + \overline{w'c'}|_{z=0},$$

if we substitute $\overline{s_c}$ by its value from equation (1), NEE reads:

$$NEE = \int_0^{z_m} \frac{\partial \overline{c}}{\partial t} dz + \int_0^{z_m} \left(\overline{u}\frac{\partial \overline{c}}{\partial x} + \overline{v}\frac{\partial \overline{c}}{\partial y} \right) dz + \\ + \int_0^{z_m} \frac{\partial \overline{w'c'}}{\partial z} dz + \overline{w'c'}|_{z=0},$$

If horizontal advection is neglected, the second right hand side term can be avoided. Moreover, taking into account the vertical linearity of the carbon dioxide fluxes showed by Casso-Torralba *et al.* (2008) for this day and also obtained with the simulations (not shown), the third integral of the right hand side is just the difference between the flux at z_m and the flux at the surface. Then, the NEE can be written as:

$$NEE = \int_0^{z_m} \frac{\partial \overline{c}}{\partial t} dz + \overline{w'c'}|_{z=z_m}. \quad (2)$$

Therefore, to calculate NEE the time evolution it's necessary to know the concentration at several heights to calculate the first right hand term of equation (2). In order words, as we showed, if equation (1) is used, the flux at several heights is needed to calculate DF. However, most of the observational sites have only measurements at one height. Therefore, to infer NEE from a point measurement the most usual approximation consists in assuming that the storage term is constant with height. This approximation is only valid in convective situations as the ones presented in the studied day. In this situation, the NEE reads:

$$NEE_0 = z_m \left(\frac{\partial \overline{c}}{\partial t} \right)_{z=z_m} + \overline{w'c'}|_{z=z_m}. \quad (3)$$

Two important remarks have to be notice. For not reactive species no sources and sinks exist for $z > 0$, then the difference of NEE_0 between two levels has to be zero. Moreover, due to the assumptions made in the MXL model

(Tennekes and Driedonks, 1982) NEE_0 is equal to the prescribed surface flux.

By using equation (3), figure 4a shows the time evolution of the NEE_0 inferred from the observations at the different measurements heights except the lowest one (solid lines), by using the DALES results at the same heights (dashed lines) and by using MXL (blue dotted line).

Before 11 UTC, some of the assumptions made for the observations are not correct because different NEE_0 are obtained from the observations for the different heights. Either the advection term cannot be neglected, either the approximation made in equation (3) regarding the well mixed boundary layer is not correct. As we show previously (figure 2c), a well mixed layer for CO_2 was observed since 10 UTC approximately. This can produce differences in the NEE_0. To analyze the influence of the MXL approximation for the observations, figure 4b shows the comparison between NEE obtained by integrating between the measurements levels (see equation 2, solid lines), and NEE_0 (dashed lines). From this figure it can be concluded that the differences in NEE between the levels are mainly due to the advection contribution. To reinforce this assumption figure 4c shows the differences in NEE between 60-100 m and 100-180 m (see Yi *et al.*, 2000). As ca be observed during the morning transition this differences are large. Only once the BL is very well mixed ΔNEE becomes small. If the wind at the different levels is analyzed (not shown) it can be concluded that direction was almost constant (120^o) during the whole day and velocity increased from 5 m s^{-1} up to 7 m s^{-1} during the early evening and only differences around 2 m s $^{-1}$ were observed between 40 and 200 m height.

Summarizing, even if the advection rate is low (see figure 3) it can contribute to the NEE calculation. Figure 4 gives a clear idea about the error that can be done in the calculation of the NEE if only a measurement height is used and the advection is neglected.

Regarding the numerical simulations, for DALES, where advection is minimum, NEE_0 is similar at the presented heights of the model equivalent to the measurement heights except for the points located at 180 m height. At this time, the simulated boundary layer with the DALES is not well mixed and the CO_2 concentration around 180 m has a different time evolution than the concentration at the lower levels (see figure 2c). For the MXL model, it can be demonstrated that the NEE_0 is equal to the prescribed CO_2 surface fluxes. However, it fits very well the observed values after 12 UTC. Both observations and simulation give negative values of the NEE_0 for this day after 12 UTC. This fact indicates that the assumption of neglected advection is correct during the studied day.

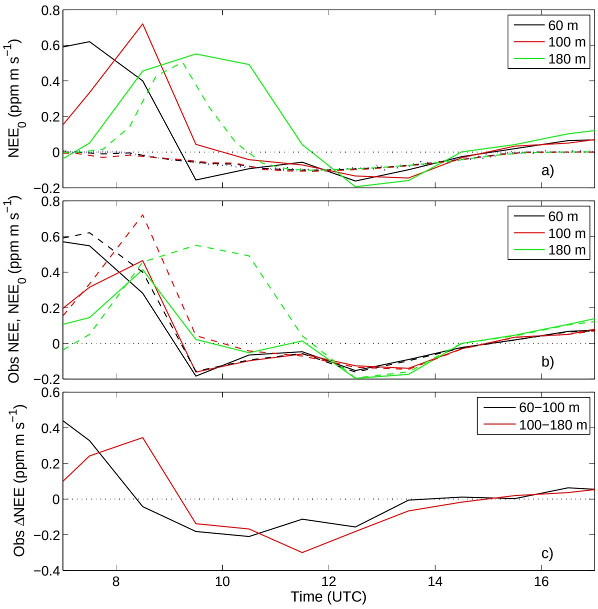

FIGURE 4: Evolution during 25th September 2003 of the (a) NEE_0 calculated by using equation (3) from the observations (solid lines), obtained by the DALES (dashed lines) at different heights and by the MXL model (blue dotted line); (b) NEE (equation 2, solid lines) and NEE_0 (equation 3, dashed lines) calculated form the observations at the three upper levels; and (c) ΔNEE between the measurements levels at 60 and 100 m (black) and between 100 and 180 m (red).

6. CONCLUSIONS

The diurnal evolution of boundary layer variables have been studied by using observations and two types of numerical simulations during a convective day. Particular attention was devoted to analyze the vertical distribution of heat and CO_2 concentration. Both the DALES and the MXL models reproduce the evolution of the bulk variables during the day.

By using the observations at four heights the heat and CO_2 budgets were analyzed. As it was already shown by Casso-Torralba *et al.* (2008), the divergence of the flux term of the budget equation (both heat and CO_2) accounts for 80-90$\%$ of the evolution of both variables. Consequently, the advection contribution was low during this day. DALES and even the simple MXL model correctly reproduce the observed evolution of the budget terms. It's important to notice the importance of the DF term specially during the morning hours where large values of entrainment were observed. This caused strong ventilation of CO_2 due to the entrained air causes the entrainment flux to be larger than the surface flux.

Particular attention has been devoted to analyze the evolution of the NEE. Even in the studied case where the advection was not important, the estimated value of the NEE at the different heights gave different results due to the advection term neglected or to the assumption of a well mixed boundary layer during the whole day. DALES and MXL, reproduce the observed values once the advection is reduced and a well mixed boundary layer is formed.

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REFERENCES

Baldocchi, D., E. Falge, L. Gu, R. Olson, D. Hollinger, S. Running, P. Anthoni, Ch. Bernhofer, K. Davis, R. Evans, J. Fuentes, A. Goldstein, G. Katul, B. Law, X. Lee, Y. Malhi, T. Meyers, W. Munger, W. Oechel, K. T. Paw U, K. Pilegaard, H. P. Schmid, R. Valentini, S. Verma, T. Vesala, K. Wilson, and S. Wofsyn, 2001: FLUXNET: A New Tool to Study the Temporal and Spatial Variability of Ecosystem-Scale Carbon Dioxide, Water Vapor, and Energy Flux Densities. *Bull. Amer. Soc.*, **82**, 2415-2434.

Beljaars, A. C. M., and F. C. Bosveld, 1997: Cabauw data for the validation of land surface parameterization schemes, *J. Clim.*, **10**, 1172-1193.

Bosveld, F. C., E. van Meijgaard, E. Moors, and C. Werner, 2004: Interpretation of flux observations along the Cabauw 200 m meteorological tower, in *16th Symp. Boundary Layers and Turbulence*, 6.18, pp. 1-4, Portland, USA.

Casso-Torralba, P., J. Vilà-Guerau de Arellano, F. Bosveld, M. R. Soler, A. Vermeulen, C. Werner, and E. Moors, 2008: Diurnal and vertical variability of the sensible heat and carbon dioxide budgets in the atmospheric surface layer. *J. Geophys. Res.*, **113**, D12119, doi:10.1029/2007JD009583.

Eugster, W., and F. Siegrist, 2000: The influence of nocturnal CO2 advection on CO_2 flux measurements*Basic Appl. Ecol.*, **1**, 177-188.

Heus, T., C. C. van Heerwaarden, H. J. J. Jonker, A. P. Siebesma, S. Axelsen, K. van den Dries, O. Geoffroy, A. F. Moene, D. Pino, S. R de Roode and J. Vilà-Guerau de Arellano, 2010: Formulation of and numerical studies with the Dutch Atmospheric Large-Eddy Simulation (DALES). *Geosci. Model Dev. Dis.*, **3**, 99-180.

Lemone, M., R. Grossman, R. McMillen, K. Liou, S. Ou, S. Mckeen, W. Angevine, K. Ikeda, and F. Chen, 2002: Cases-97: Late-morning warming and moistening of the convective boundary layer over the Walnut River watershed, *Bound.-Lay. Meteorol.*, **104(1)**, 1-52.

Pino, D., J. Vilà-Guerau de Arellano and S. –W. Kim, 2006: Representing sheared convective boundary layer by zeroth- and first-order-jump mixed layer models: Large–eddy simulation verification. *J. Appl. Meteor. Clim.*, **45,** 1224-1243.

Tenekes, H. and A. G. M. Driedonks, 1981: Basic entrainment equations for the atmospheric boundary layer. *Bound.-Lay. Meteorol.*, **20**, 515-531.

Valentini R., G. Matteucci, A. J. Dolman, E- -D. Schulze, C. Rebmann, E. J. Moors, A. Granier, P. Gross, N. O. Jensen, K. Pilegaard, A. Lindroth, A. Grelle, C. Bernhofer, T. T. Grünwald, M. Aubinet, R. Ceulemans, A. S. Kowalski, T. Vesala, Ü Rannik, P. Berbigier, D. Loustau, J. Gudmundsson, H. Thorgeirsson, A. Ibrom, K. Morgenstern, R. Clement, J. Moncrieff, L. Montagnani, S. Minerbi, P. G. Jarvis, 2000: Respiration as the main determinant of carbon balance in European forests. *Nature*, **404**, 861-865.

Vilà-Guerau de Arellano, J., B. Gioli, F. Miglietta, H. Jonker, H. Baltink, R. Hutjes, and A. Holtslag, 2004: Entrainment process of carbon dioxide in the atmospheric boundary layer, *J. Geophys. Res.*, **109**, D18110, doi:10.1029/2004JD004725.

Yi, C., K. Davis, P. Bakwin, B. Berger, and L. C. Marr, 2000: Influence of advection on measurements of the net ecosystem-atmosphere exchange of CO2 from a very tall tower, *J. Geophys Res.*, **105(D8)**, 9991-9999.