Surface heterogeneity and its signature in higher-order scalar similarity relationships

M. Detto,*, G. Katul, M. Mancini, N. Montaldo, J.D. Albertson

aDepartment of Environmental Science, Policy, and Management (ESPM), University of California, 105 Hilgard Hall, Berkeley, CA 94720, USA
bNicholas School of the Environment and Earth Sciences, Duke University, Durham, NC, USA
cDepartment of Civil and Environmental Engineering, Pratt School of Engineering, Duke University, Durham, NC, USA
dDipartimento di Ingegneria Idraulica, Ambientale e del Rilevamento, Politecnico di Milano, Italy

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ABSTRACT

Over the past three decades, a number of field experiments have suggested that land-cover heterogeneity (LCH) impacts Monin and Obukhov (M–O) scaling, when applied to second-order statistics of temperature (T), water vapor (q), and CO₂ (c) fluctuations. To further explore how LCH modifies M–O scaling for second-order statistics, 2 years of atmospheric surface layer (ASL) measurements, conducted above a Mediterranean ecosystem in Sardinia, Italy were analyzed. During wet soil moisture states, when grass and trees dominate the ecosystem, M–O similarity theory predictions significantly underestimated all three scalar variance measurements, consistent with several recent studies. Among the three scalars, q was poorly predicted by M–O scaling despite its ground source/sink similarity with c. A plausible explanation for the de-correlation between q and c is the dissimilarities originating from the top of the boundary layer via entrainment processes. To establish necessary (but not sufficient) conditions that diagnose departures from M–O scaling, the statistical structure of LCH as quantified by its integral length scale (Lx), computed using the NDVI obtained from QuickBird imagery, was employed. When the ecosystem was dominated by grass and trees (wet soil moisture states), Lx ≈ 100 m, and when the ecosystem was dominated by soil and trees (dry soil moisture states), Lx ≈ 10 m. Using the scalar variance budget equation, two canonical time scales connected with the advection–distortion and relaxation time scales were introduced in the absence of flux-transport terms. We showed that M–O scaling is recovered when relaxation time scales of turbulent eddies are much smaller than the advection–distortion time scale by the mean flow (whose length scale was set to Lx). Converting these time scales to approximate length scales, we found that a necessary but not sufficient condition for MOST to be applicable to second-order scalar statistics is when Lx ≫ zₘ(u*/u), where κ is the von-Karman constant, zₘ is the measurement height, u is the mean wind speed, and u* is the friction velocity. The term κzₑ(u*/u) did not vary considerably between the two seasons. Its value (on average 20 m) was comparable to Lx for the tree–soil system but an order of magnitude smaller than Lx for the tree–grass system.

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* Corresponding author. Tel.: +1 510 643 7430; fax: +1 510 643 543.
E-mail address: mdetto@nature.berkeley.edu (M. Detto).
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1. Introduction

Monin–Obukhov similarity theory (MOST) is widely used to link surface fluxes to the mean meteorological states in the atmospheric surface layer (ASL)—often via bulk transfer coefficients (Brutsaert, 1982). M–O scaling is also used to relate second-order turbulence moments to surface fluxes, an approach now referred to as flux-variance (FV) scaling (e.g. Tillman, 1972; Wesley, 1988; Lloyd et al., 1991; Weaver, 1990). The FV is now widely used to explore similarities in sources and sinks at the ground surface (Hill, 1989; Padro, 1993), or to quantify similarities in turbulent transport efficiencies (or turbulent diffusive properties) of various scalars (e.g. temperature, water vapor, and CO2) originating from the land surface (McBean and Miyake, 1972; Asanuma and Brutsaert, 1999; De Bruin et al., 1993; Katul and Hsieh, 1997; Lamaud and Irvine, 2006). More recently, FV was proposed as a tool to constrain and gap-fill long-term CO2 flux data (Choi et al., 2004) and to assess the quality of eddy correlation flux measurements (Foken and Wichura, 1996).

Over the past 20 years, several ASL experiments over heterogeneous surfaces have documented dissimilarity in the vertical transfer of sensible heat and water vapor, as well as in their respective FV functions (Lamaud and Irvine, 2006; Lyons and Halldin, 2004). Though the linkage remains qualitative, it is often argued that departures from MOST predictions can be linked to some statistical attribute of the heterogeneity of source/sink distribution at the land surface (Andreas et al., 1998; Katul et al., 1995; Kustas et al., 1994; Lamaud and Irvine, 2006; Padro, 1993; Wesson et al., 2001).

Due to recent advancements in remote sensing, accurate maps of vegetation index (e.g. NDVI) with 1 m by 1 m resolution, can now permit the quantification of small scale land-cover heterogeneity (LCH) (e.g. Scanlon et al., 2007). At the same time, refinements in 2-D foot print models (Detto et al., 2006; Klijun et al., 2002) can now identify the source area of the tower based flux measurements. The unprecedented land-surface cover data and analyzing tools, in conjunction with long-term turbulent statistics, are now allowing systematic inspection of how LCH (in NDVI) might impact M–O scaling.

Our overall objective is to derive rule-of-thumb measures that provide diagnostics as to whether MOST FV relations apply to a particular landscape based on the spatial organization of NDVI, sampled by high-resolution remote sensing products. A first step to progress on this objective is to systematically investigate how LCH impacts M–O scaling for higher-order turbulent scalar quantities measured in the ASL. LCH effects can rise from both diurnal shifts in the source-weight function on short time scales, and also in ecosystem composition on seasonal time scales.

With these two time scales in mind, the main novelties in the experimental setup are two-fold. (1) Unlike earlier studies that primarily focused on two scalars – temperature (an active scalar in terms of buoyant production/dissipation of turbulent kinetic energy) and water vapor, the setup here included a third scalar – CO2. This passive gas has the added advantage of providing an independent quantity originating from sources/sinks spatially co-located with the evaporative sources, but affected by meso-scale modulations that can be different from the ones that affect heat and water vapour (e.g. entrainment from the top of the atmospheric boundary layer). (2) The landscape composition significantly changes with the hydrologic regime thereby permitting a wide range of landscape structure and function to be sampled from the same meteorological tower.

2. Experiment

Much of the experimental setup is presented in Detto et al. (2006), but salient features are reviewed for completeness.

2.1. The site

The experiment was conducted in Orroli (Italy), which is situated in mid-western Sardinia (39°41’12.57"N, 9°6’30.34"E, 500 m s.l.m.). The landscape is a mixture of Mediterranean patchy vegetation types: trees including wild olives and cork oaks; and different shrubs and herbaceous species that are present only during wet seasons. The bare soil is the dominant land-cover (more than 70% on a fractional area basis) during the summer. The trees (maximum tree height h<sub>t</sub> < 5 m) and their foliage density remain approximately constant throughout the year (woody leaf area index, LAI, fluctuates between 3.5 and 4.5), whereas the herbaceous leaf area rapidly increases from zero to a maximum LAI = 2 with winter and spring. Precipitation is almost absent in the summer. Hence, throughout, wet soil moisture states (mainly in the winter-spring period) refers to the grass–tree ecosystems, and dry soil moisture states (mainly in the summer period), to soil–tree ecosystems.

2.2. The meteorological and hydrological measurements

An eddy-covariance system equipped with a Campbell Scientific CSAT-3 sonic anemometer and Licor-7500 CO2/H2O infrared gas analyzer was used to measure the velocity and scalar concentration in the atmospheric surface layer at 10 m above the ground surface. The data collection commenced on April of 2003 as part of a long-term water vapor and CO2 flux monitoring initiative, and the period analyzed here extends up to October of 2005. Half hourly statistics (i.e. means, variances, and co-variances) between the three velocity components (u, v and w), air temperature T, specific humidity q, and carbon dioxide density c were computed from 10 Hz series sampled by a CR23X data logger (Campbell Scientific). During the processing of the statistics, the acquisition logger program excluded possible bad values due to electrical spikes. Throughout, u(or u<sub>L</sub>) is the velocity component along the longitudinal (x or x<sub>L</sub>) or mean wind direction, v (or u<sub>W</sub>) is the velocity component along the lateral direction (y or x<sub>L</sub>), and w is the velocity component along the vertical direction (z or x<sub>W</sub>). With a measurement height at least two times the maximum canopy height, it was assumed throughout that the data is being collected above the roughness sublayer (Raupach et al., 1996). Seven frequency domain reflectometer probes (FDR Campbell CS615) were installed, both vertically and horizontally, to measure the mean soil moisture content within the root-zone thereby informing on surface aridity.
2.3. Remote sensing image

Two multispectral (VIS and NIR) high spatial resolution (pixel size: 2.8 m × 2.8 m) Quickbird satellite images, acquired in 2004 on DOY = 220, 2003 and DOY = 138 were used to retrieve the tree cover map via a supervised classification scheme based on the parallelepiped algorithm (Richards, 1999). The NDVI (NIR – R/NIR + R) values were subsequently computed on a 2.8 m by 2.8 m resolution, where NIR and R are the near-infra and red bands, respectively.

2.4. Post-processing

The first step in post-processing the eddy-covariance data is a coordinate rotation. We used a variant on the planar fit method (Lee et al., 2004) so that the mean lateral velocity was zero for each 1/2 hourly run. However, the ensemble-averaged vertical velocity was used to correct the tilt angle for each wind direction (see Appendix A).

Sensible heat flux corrections for the open-path measured scalar density fluctuations were also applied to water vapor and CO₂ variances and their co-variances with vertical velocity (Webb et al., 1980) approach described in Detto and Katul and other scalars. The scalar density corrections were derived using an recent extension of the Webb–Pearman–Leuning (WPL) (Webb et al., 1980) approach described in Detto and Katul (2007). These corrections, summarized in Appendix B for completeness, are compact formulations that can be employed for post-processing variances and covariances. For the vertical turbulent flux of c or q, these corrections reduce to the standard WPL.

Only daytime runs for which vertical fluxes were bounded by physically realistic values were employed. Runs during rainfall events, strong subsidence, and low wind speed conditions were excluded. The data filtering thresholds, shown in Table 1, reduced the number of 1/2 hourly runs from a maximum possible 35,399 (day and night) to 6282 (daytime only).

3. Theory

3.1. The flux-variance method (FVM)

Based on MOST, any dimensionless turbulence statistic depends on the atmospheric stability parameter, \( \zeta = z/L \), where \( z \) is the height above the zero-plane displacement, and \( L \) is the Obukhov (Stull, 1988).

The turbulent variance of any scalar \( s \), \( \sigma_s^2 \), can be expressed as a function of \( \zeta \) using

\[
\frac{\sigma_s^2}{\bar{s}^2} = -\phi_s(\zeta)
\]  

(1)

where \( s = -\overline{wu}/u_* \) is a turbulent scalar concentration scale; \( \overline{wu} \) is the vertical flux and \( u_* \) is the friction velocity given by

\[
u_* = \left(\overline{u^2} + \overline{w'^2}\right)^{1/2},
\]

(2)

where \( u', w', \) and \( v' \) are the turbulent fluctuations in the longitudinal, vertical, and lateral velocities, respectively.

The function \( \phi_s(\zeta) \) must satisfy two limits (e.g. Garratt, 1992):

(1) In the neutral case, \( -\xi \to 0 \) and \( \phi_s(-\xi) \) approaches a constant.

(2) In the free convection limit, \( -\xi \to \infty \) and \( \sigma_s/\bar{s} \) should become independent of \( u_* \).

These two limits can be satisfied with the expression

\[
\frac{\sigma_s^2}{\bar{s}^2} = -C_1(1 - C_2\xi)^{-1/3}
\]

(3)

where \( C_1 \) and \( C_2 \) are similarity constants (e.g. Stull, 1988; Sorbjan, 1989).

For the free convection conditions (e.g. \( -\zeta > 5 \)), Eq. (3) is well approximated by

\[
\frac{\sigma_s^2}{\bar{s}^2} \approx -C_3(1 - \xi)^{-1/3}
\]

(4)

where \( C_3 \approx 0.99 \) (corrected for \( \kappa = 0.4 \)) was originally determined in Wyngaard et al. (1971) and verified over a uniform and flat dry lakebed by (Albertson et al., 1995) and for several canopies by (Wesson et al., 2001). For homogeneous conditions, \( \phi_s(\xi) \) was shown experimentally (over a uniform wheat field) to be the same for heat, water vapor, and CO₂ (Ohtaki, 1992).

3.2. Scalar variance budgets

The processes affecting \( \sigma_s \) can be formally studied via the scalar variance budget equation, which for an incompressible and high Reynolds number flow, is given by (Garratt, 1992)

\[
\frac{\partial \sigma_s^2}{\partial t} + \overline{u_j \frac{\partial \sigma_s^2}{\partial x_j}} = -2\overline{u_i \frac{\partial \sigma_s}{\partial x_i} \frac{\partial \sigma_s}{\partial x_j}} - 2\overline{s_s \frac{\partial \bar{s}}{\partial x_j}},
\]

(5)

where term I is the local rate of change of the scalar variance, term II is the advection of the scalar variance, term III is the scalar variance production term by the mean scalar gradient, term IV is the scalar variance flux transport, and term V (or \( \overline{\epsilon_s} \)) is the scalar variance dissipation. Assuming stationary conditions (\( \partial i/\partial t = 0 \), rotating the coordinate
axes so that the lateral component $\bar{u}_2 = \bar{v} = 0$, and selecting runs in which subsidence can be neglected ($\bar{u}_3 = \bar{w} = 0$), the resulting two-dimensional variance budget equation reduces to:

$$\frac{\partial \overline{u^2_s}}{\partial x} = -2\overline{u'u'_{s}}\frac{\partial \bar{u}}{\partial x} - 2\overline{u'u'_{s}}\frac{\partial \bar{v}}{\partial z} - 2\varepsilon_s - TR. \quad (6)$$

where $TR = \partial/\partial z(\overline{u'u'_{s}}/\bar{u}) + \partial/\partial y(\overline{v'v'_{s}}/\bar{v}) + \partial/\partial z(\overline{w'w'_{s}}/\bar{w})$.

In the context of Eq. (6), M–O scaling assumptions further require a planar homogeneous (i.e. $\partial \bar{u}/\partial x = \partial \bar{v}/\partial y = 0$) flow (i.e. no longitudinal length scale is present in M–O scaling). Furthermore, if a simplified second-order closure expression for TR, given by $TR = \partial/\partial z(\overline{u'u'_{s}}/\bar{u}) \sim \partial/\partial z(\tau/C_4 \overline{u'u'_{s}}/\partial z \overline{u'u'_{s}} + \ldots)$ is assumed, then $C_4$ is a similarity constant and $\tau$ is the relaxation time scale defined later (see Siqueira and Katul, 2002), TR can be neglected because $\partial \bar{u}/\partial z \overline{u'u'_{s}} \approx 0$ (i.e. the constant scalar flux with height is a requirement of M–O scaling).

With these assumptions, Eq. (6) results in a balance between turbulent production and dissipation given as

$$-\overline{u'u'_{s}}\frac{\partial \bar{u}}{\partial z} = \varepsilon_s. \quad (7)$$

This simplified budget in Eq. (7) was used by numerous investigators to estimate scalar variance dissipation rates in the ASL (e.g. Wyngaard and Coté, 1971; Champagne et al., 1977; Panofsky and Dutton, 1984; Fairall and Larsen, 1986; Kader and Yaglom, 1990) and forms the basis of two recent dissipation rate methods reviewed in Albertson et al. (1997) and Hsieh and Katul (1997). It is now possible to derive the ‘standard’ flux-variance similarity function by using higher-order closure principles to relate $\varepsilon_s$ to $\varepsilon_s$ using (e.g. Siqueira et al., 2002)

$$\varepsilon_s = \frac{C_\varepsilon}{\tau} \sigma_s^2 \quad (8)$$

where $\tau = \bar{u}'/\varepsilon_{\text{TKE}} = kz/\bar{u}$, $\phi_{\text{TKE}}(\zeta)/\phi_s(\zeta)$ is, as before, a relaxation time scale, $\varepsilon_{\text{TKE}}$ is the mean turbulent kinetic energy (TKE) dissipation rate, $\phi_{\text{TKE}}$ and $\phi_s(\zeta)$ are the ASL stability correction functions for the TKE and $\varepsilon_{\text{TKE}}$, respectively, and $C_\varepsilon$ is a closure constant (Siqueira et al., 2002). Substituting it in Eq. (8), the stability correction function of the variance dissipation (or production), $\phi_{\varepsilon_s}$ is given by:

$$\phi_{\varepsilon_s} = \frac{kz}{\bar{u}} \frac{\sigma_s^2}{\bar{s}^2} \phi_{\text{TKE}}$$

From the three-sublayer model of (Kader and Yaglom, 1990) for ASL flows (Kader, 1992), and (Hsieh and Katul, 1997) showed that:

$$\phi = 0.5(8.5 + \phi_{\varepsilon_s})$$

$$\phi_{\varepsilon_s} = 0.4\left(\frac{10 + 7.5(-\zeta) + 6.25(-\zeta)^2}{4 + 2.5(-\zeta)}\right)^{1/3}$$

resulting in

$$\phi_s = \sqrt{\frac{1}{C_\varepsilon} \phi_{\text{TKE}} \phi_{\varepsilon_s}} \quad (9)$$

That is, the FV similarity functions for scalars can be inferred from M–O velocity and dissipation stability correction functions. Note that except for near-neutral conditions, the three Eqs. (4), (5) and (9), agree reasonably well with each other. This agreement suggests that the only relevant time scale for the variance budget equation to reproduce M–O scaling (for FV predictions) is the relaxation time scale $\tau$.

### 3.3. Scaling arguments for the variance budget

It is not our intent here to measure or analyze all the individual components of the scalar variance budget in Eq. (7); instead, we illustrate how horizontal gradients, introduced by LCH, may modify M–O FV scaling primarily by disrupting the balance between scalar variance production and its dissipation rate. Eq. (7) suggests the imbalance between production and dissipation can be traced back to three terms: $\overline{u'u'_{s}}\overline{\sigma_{\bar{u}}}/\bar{u}$, $\overline{u'u'_{s}}\overline{\sigma_{\bar{v}}}/\bar{v}$, and TR. While the genesis of the two terms $(\overline{u'u'_{s}}\overline{\sigma_{\bar{u}}}/\bar{u}, \overline{u'u'_{s}}\overline{\sigma_{\bar{v}}}/\bar{v})$ is from the existence of stream-wise gradients, the TR terms (at least one of them) need not be. For example, the TR terms become important if entrainment fluxes from the capping inversion can be communicated down to the ASL (e.g. De Bruin et al., 1993; Roth and Oke, 1995). Recently, Katul et al. (2008) presented an analytical solution demonstrating how this term introduces a de-correlation between $T$ and $q$ in the marine ASL.

However, it is safe to say that the two advective terms in Eq. (7) become important when $l_s$ is comparable to $\kappa z$.

Qualitatively, this statement is supported by the following scaling arguments: let $\partial \bar{u}/\partial x \sim (\bar{u}/l_x, \partial \bar{u}/\partial z \sim \bar{u}/l_z, \sigma_{\bar{u}} \sim s^2$ (i.e. using the FV approach), and $\overline{u'u'_{s}} = \bar{u}u_s$. Using these two length and concentration scales, the order of magnitude of the two advective terms in Eq. (7) becomes

$$\overline{u'u'_{s}}\overline{\sigma_{\bar{u}}}/\bar{u} \sim \overline{u'u'_{s}}\overline{\sigma_{\bar{u}}}/l_x$$

and

$$\overline{u'u'_{s}}\overline{\sigma_{\bar{u}}}/\bar{u} \sim \overline{u'u'_{s}}\overline{\sigma_{\bar{u}}}/l_x$$

while the production term is given by M–O scaling:

$$\overline{u'u'_{s}}\overline{\sigma_{\bar{u}}}/\bar{u} \sim \overline{u'u'_{s}}/l_x$$

Hence, the relative importance of these two advective terms to the production term is:

$$\overline{u'u'_{s}}\overline{\sigma_{\bar{u}}}/\bar{u} \sim \overline{u'u'_{s}}/l_x \sim \kappa z \overline{u}/l_x$$

and

$$\overline{u'u'_{s}}\overline{\sigma_{\bar{u}}}/\bar{u} \sim \overline{u'u'_{s}}/l_x \sim \kappa z \overline{u}/l_x$$
When $L_m \gg \zeta$, the importance of the two advective terms significantly diminishes (for a uniform terrain, $L_m \to \infty$). In the ASL, $\tau / u_* \sim \log(z_{om}/z_{om}) > \nu_{om}^2 \zeta / u_* s_\xi$, at least for measurement heights ($z_{om} \sim 10$ m) much larger than the momentum roughness length ($z_{om} \sim 0.7$ m) as is the case here. However, this assumption can be tested from single-tower measurements. If so, then $\nu_{om}^2 \zeta / u_* s_\xi < 10 u_* \alpha z_{om}$ and only one of these two advective terms need be considered. Not notwithstanding this argument, when turbulent horizontal transport efficiencies and FV dissimilarities among scalars are being evaluated, the dissimilarities in $\nu_{om}$ should be considered.

4. Results

The main statistical features of the LCH are first described using the two NDVI maps obtained from the Quickbird satellite. How the tower samples this NDVI variability is then analyzed via a two-dimensional footprint model for each atmospheric stability class and for each wind direction cluster. Lastly, the signature of NDVI heterogeneity on FV relations and other higher-order scalar moments at short time scales (e.g. changes in atmospheric stability) and seasonal time scales (e.g. ecosystem composition changes) are shown. Rule-of-thumb scaling rules are then proposed and verified using the analysis in Section 4.3 when $\nu_{om}^2 \zeta / u_* s_\xi < 10 u_* \alpha z_{om}$ and in the absence of significant TR.

4.1. Land-cover heterogeneity

Fig. 1 shows the spatial variation in NDVI (normalized by its maximum value) in a 1 km by 1 km square patch surrounding the tower for both summer and spring seasons. The dimensionless NDVI variability can be used as a surrogate for scalar source–sink strength variability because in these sparsely vegetated Mediterranean ecosystems, LAI is sufficiently low so that an NDVI versus LAI relationship remains approximately linear (i.e. far from saturation). From Fig. 1, it is evident that for summertime conditions, the mean NDVI in the North–East (NW) and South–West (SE) quadrants is, on average, higher than the South–East (SW) and North–West (NE) quadrants demonstrating clear anisotropy in vegetation cover distribution. To average out this anisotropy, a two-dimensional autocorrelation function of NDVI for both images, also shown in Fig. 1, is used to compute the effective integral length scale of NDVI variability ($L_m$). The computed $L_m$ is on the order of 10 m for the bare soil–tree components and is on the order of 100 m for the tree–grass components. For the bare soil–tree configuration, $L_m = 10$ m is comparable to the size of attached eddies ($\sim \zeta x$) and hence may well interact with the vertical transfer as noted in Section 4.3. The spatial average of NDVI as a function of radial distance ($r$) originating from the tower becomes independent of $r$ at $r = 600$ m, roughly coinciding with the mean distance between large tree clusters (Fig. 1e) for the bare soil–tree configuration. This length scale is also dynamically important because it is comparable to the (1) crosswind integrated footprint size for neutral conditions; and (2) convective boundary layer depth (with possible implications to TR).

While the NDVI spatial variability within the 1 km by 1 km may be stationary within a given season, the 1/2 hourly variability in wind direction, sensible heat flux, and friction velocity, ensures that the tower measurements do not sample uniformly this NDVI spatial variance.

4.2. Linking the tree distribution to the tower-based meteorological measurements

A 2-D footprint analysis was conducted to assess the dependence of the sampled NDVI (computed only for trees as in Fig. 1a) at the tower on atmospheric stability conditions and wind direction. The footprint model employed is an extension of an earlier analytical model (Hsieh et al., 2000), but now includes lateral dispersion using the tower-measured $\alpha_w$ (Detto et al., 2006). In addition to the flow statistics and sensible heat flux, the footprint model requires the wind direction and $z_{om}$ to be specified. The latter was determined directly from near-neutral atmospheric stability runs ($z_{om} \approx 0.7$ m) for different wind directions.

This 2-D footprint function ($f = f(x, y)$) is used to evaluate the weighted NDVI using

$$\text{NDVI}_f = \int_A f(x, y) \text{NDVI}(x, y) dA \quad (9)$$

Eq. (9) was solved numerically by discretizing the above integral on the NDVI digital image collected during the dry period (Fig. 1a), where the NDVI of the bare soil was set to zero.

Based on these model calculations for the soil–tree configuration (used as illustration), we found that when $\zeta$ approaches convective conditions, the footprint weighted NDVI becomes large (see mode in Fig. 2, top panel). This large NDVI is primarily due to the fact that the footprint size is small and samples no more than 50 m from the tower. As shown in Fig. 1e, the NDVI at $r = 50$ m is near its maximum value. In contrast, when $\zeta$ is small (i.e. near-neutral), the footprint size is sufficiently large to sample significant bare soil spots (Fig. 2, top). The emergence of two modes in the footprint weighted NDVI are primarily due to the bimodality in wind direction (see Fig. 2, bottom). Besides these modes, it is clear from Fig. 2 that within each stability class, a broad range of NDVI values is being sampled. The specific signature of this NDVI variability in FV similarity relationships for each stability class is explored next.

4.3. Impact of LCH on FV and higher-order moments

The measured FV similarity functions for vertical velocity $\phi_w$, heat $\phi_q$, water vapor $\phi_w$, and CO$_2$ $\phi_c$ as a function of $\zeta$ are first reported for wet, intermediate, and dry soil moisture states in Figs. 3 and 4. The $\phi_w, \phi_q, \phi_w, \phi_c$ here were not strictly in the ASL because $2 < z_{om}/h_c < 10$, and hence, some modulations to the flow statistics from the canopy sublayer cannot be entirely excluded (Raupach and Thom, 1981). In fact, the flow just above a rough surface is strongly influenced by the geometry of the roughness elements through “wake diffusion” effects, but also through the spatial distributions of sources and sinks (Raupach and Thom, 1981). Using vertical velocity spectra collected from Laser-Doppler Anemometry, Poggi et al. (2004) showed that the effects of these wakes (on wake production) extend up to 1.2 $h_c$ from the ground for a canopy composed of densely arrayed rods. However, no study to date considered the effects of such wakes on scalar diffusion.
4.3.1. Vertical velocity
Despite the wide range of variability in NDVI sampled within each stability class, agreement between M–O scaling for $\phi_w$ and the measurements here is surprisingly good (Fig. 3). Specifically, when the canonical M–O function for $\phi_w$, given by

$$\phi_w = A_1 \left(1 - A_2 \zeta \right)^{1/3}$$

is fitted to the entire data set (i.e. $n = 6282$, 30-min runs) using least-squares analysis, the resulting $A_1 = 1.2$ and $A_2 = 2$. These values are smaller than those reported in Panofsky and Dutton (1984) (i.e. $A_1 = 1.25$ and $A_2 = 3$) but are within the range of other data sets (Pahlow et al., 2001). Hence, the small scatter in Fig. 3 suggests that NDVI variability, while large within each stability class, does not significantly impact the vertical velocity $FV$ relationship, even when the ecosystem changes composition (i.e. from grass–tree to soil–tree states).

4.3.2. Scalar statistics
As discussed in Detto et al. (2006), the contrast in skin temperature between the trees and bare soil is much larger than the contrast in skin temperature between the trees and...
When contrasting the three hydrologic states (wet, intermediate, and dry), the departure between measured $\phi_T, \phi_q, \phi_c$ from their M–O similarity values at a given $\zeta$ decreases with increasing soil moisture. Surprisingly, the departure between measured and M–O similarity theory predicted $\phi_c$ is smaller than its $\phi_q$ counterpart for dry conditions. Given the intimate link between photosynthesis and transpiration at this site, the fact that $\phi_q > \phi_c$ for dry conditions suggests that surface heterogeneity alone may not explain all the departures from M–O scaling (De Bruin et al., 1993). The data here is insufficient to strictly explore whether entrainment from the top of the atmospheric boundary layer is responsible for $\phi_q > \phi_c$ as proposed in other studies for heat and water vapor (De Bruin et al., 1993; Johansson et al., 2001) though some indirect evidence may be extracted when analyzing correlations among the three scalars for different soil moisture states.

In Fig. 5, the similarity in turbulent transport efficiencies between heat and the remaining two scalars for wet, intermediate, and dry soil moisture conditions is explored. For wet conditions, the similarity between $T'$ and $q'$ or $c'$ remains significantly high (see modes in Fig. 5a and b), consistent with the analysis in Fig. 4 and the recent analysis by Lamaud and Irvine (2006). For dry conditions, the similarity breaks down for $T'$ and $c'$, while the scatter significantly increases for $T'$ and $q'$ (though the mode is not as shifted as the mode in the $T'$–$c'$ analysis). The histograms in Fig. 5c and d suggest clear weakening in the transport efficiency for dry conditions while for wet conditions the transport efficiency is consistent with MOST for both scalars (see the modes in Fig. 5c and d). This shift indicates that for the dry state—a de-correlation between $w'$ and scalar concentration fluctuation must have occurred, at least with respect to the wet soil moisture conditions, also consistent with the analysis in Lamaud and Irvine (2006) (although their heterogeneity is vertical not planar). In Lamaud and Irvine (2006), they presented this de-correlation with respect to an increase in the Bowen ratio rather than a decrease in soil moisture.

4.4. Entrainment and indirect diagnostic on the TR term

For the dry soil moisture states, the bare soil is a large source of heat while the vegetation is not. The fact that the heat sources and water vapor sources (or CO$_2$ sinks) are no spatially co-located contributes to the dissimilarity between heat and the remaining two scalars. Hence, entrainment processes may not be well resolved by the dissimilarity in $q'$ and $T'$ here. However, the trees remain the only ground source of water vapor and sink for CO$_2$ (except for low photosynthetically active radiation, where plant respiration may become significant). It follows that by exploring the transport efficiencies of $c'$ and $q'$ for the three soil moisture states, it may be possible to infer whether modulations of the ASL originating from the outer layer are occurring given the source–sink similarities (i.e. trees) at the ground for these two scalars. We also note that $c'$ and $q'$ are both almost passive scalars (Katul and Hsieh, 1999). Fig. 6 shows the histogram of the correlation coefficient between $c'$ and $q'$ for the three hydrologic states. For wet conditions, the similarity in transport efficiency is around 0.9 consistent with MOST predictions (i.e. unity). For intermediate soil moisture states, the mode in the correlation remains near...
Fig. 3 – Flux-variance relationship for the vertical velocity as function of stability for the three hydrological conditions. The least-squares fit and the Panofsky and Dutton (1984) functions are also shown.

Fig. 4 – Flux-variance relationships for temperature, water vapor and CO₂ as function of stability for the three hydrological conditions. The similarity parameters are $C_1 = 2.7$ and $C_2 = 12$, in Eq. (9) $C_5 = 0.8$. 
Fig. 5 – Distribution functions of the correlation coefficients between water vapor and CO₂ with temperature (Top), and between water vapor and CO₂ with vertical velocity (Bottom).

Fig. 6 – Distribution functions of the correlation coefficient between water vapor and CO₂. The inset shows the correlation coefficients for high and low photosynthetically active radiation (PAR) demonstrating the strong negative correlation occurring frequently at high PAR while positive correlations occurring frequently at low PAR.
unity but the scatter increases. Finally, for the dry soil moisture state, the correlation drops by a factor of 2. Hence, despite the similarity in sources and sinks at the ground for $c'$ and $q'$, their transport efficiency is significantly different under dry soil moisture states. Plausible explanations for this difference in transport efficiency often invoke entrainment processes modulating the ASL. For example, Roth and Oke (1995) argued that in a dry and deep convective boundary layer, thermals are sufficiently energetic to penetrate the capping inversion thereby rapidly transporting down to the surface any 'inverse' correlation between $q'$ and $T'$. This top-down transport has the effect of further weakening the correlation between temperature and humidity—especially when the ground humidity source is already low relative to heat. It was already shown, in fact, using aircraft measurements performed above the Landes forest, that this anti-correlation between $q'$ and $T'$ was most likely to occur when the surface evaporation was weak (Mahrt, 1991).

The availability of three scalars permits assessing how entrainment processes might modulate correlation coefficients between $q'$ and $T'$, $c'$ and $q'$, and $c'$ and $T'$ assuming that at the top of the ABL, CO$_2$ and water vapour are depleted while the temperature is warmer near the capping inversion. The warmer temperature and depleted humidity have been documented in capping inversion studies (Mahrt, 1991); however, less is known about CO$_2$. Recently, de Arellano et al. (2004) found that CO$_2$ concentrations are depleted above the capping inversion at Cabauw (the Netherlands) during the growth of the ABL. Noting that Sardinia is an island with low population density and is lacking any industry emitting anthropogenic carbon gases, it is plausible that CO$_2$ concentrations above the capping inversion are also depleted.

This combination of scalar correlations above the capping inversion may explain the strength of the correlation between $c'$ and $q'$ in the ASL if we assume that the capping inversion scalar correlations are transmitted to the ASL by a top-down diffusion without any distortion. Based on this hypothesis, one can explain why during dry soil moisture states, $|R_{TC}| > |R_{Tq}|$ and $|R_{tcq}| < 1$ as illustrated in Fig. 7 with quadrant analysis. Fig. 7 schematically shows how inhomogeneity, originating from the dry soil and entrainment, might affect the correlations among the three scalars and departures from M–O scaling predictions (i.e. 1:1 line). For the correlation between $T'$ and $q'$, inhomogeneity and entrainment both contribute to a quadrant that significantly reduce their correlation. For $T'$ and $c'$, only inhomogeneity contributes to the quadrant producing the de-correlation, while for $q'$ and $c'$ only entrainment contributes to the quadrant producing a de-correlation in this experimental setup. The emerging picture from Fig. 7 is that (i) $|R_{tcq}| < 1$ primarily due to entrainment and other modulations from the outer layer, (ii) $|R_{TC}| > |R_{Tq}|$ can be explained by the fact that $|R_{Tq}|$ is impacted by both—entrainment and LCH while $|R_{TC}|$ is only impacted by entrainment and other outer-layer modulations. These inequalities in correlations are consistent with the modes of the pdf measurements reported in Figs. 5 and 6 for dry soil moisture states.

4.4.1. Turbulent variance transport

As noted in Section 4.3, the variance budget suggests that $u^2$ can generate a new term that disrupts the balance between

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**Fig. 7** – Conceptual framework of how entrainment and surface heterogeneity might impact the correlation coefficients among the three scalars. Scalar correlations above the atmospheric boundary layer are assumed to propagate without alterations to the ASL. In the quadrant analysis shown, the dashed lines are MOST predictions, shaded gray areas around MOST predictions are expected measurements without any alterations from entrainment and/or surface heterogeneity, solid gray and black represent the quadrants most likely to experience entrainment and surface heterogeneity signatures, respectively. Maximum scalar de-correlation occurs if entrainment and or surface heterogeneity contribute to quadrants opposite to the quadrants populated by MOST.
scalar variance production and its dissipation thereby amplifying dissimilarity amongst observed FV functions. In Fig. 8, we show the variations of $c_1s = u_0s_0$ for both wet and dry periods. Interestingly, the highest scatter appears for $c_1q$ for dry conditions (and for near-neutral state) consistent with the analysis in Fig. 4. Furthermore, the dependence of $c_1q$ on $z$ is much higher when compared to $c_1c$ and $c_1q$ irrespective of the soil moisture state. This analysis, when combined with the scaling argument in Section 4.3, suggests that differences in $u_0s_0$ can explain why $f_q > f_c$, especially for the near-neutral conditions. Note that $|c_1q|$ for dry soil moisture states is not small ($\leq 0.24$) for near-neutral conditions and may be comparable to $\bar{u}/u_*$, which we investigate later. This is not an issue in convective conditions in which the covariance $\bar{u}s$ vanishes.

5. Discussion

Why MOST predictions diverged from the measurements in Figs. 4–8 for dry soil moisture states are not due to a singular reason. From the variance budget equation, three plausible reasons have been identified: $\bar{u}s_s\partial s/\partial x$, $u\bar{s}_s^2/\partial x$, and TR. The first two can be linked with a horizontal length scale describing variability in NDVI, while TR is likely to be linked with entrainment processes. Scaling arguments suggest that when $u/u_* \gg |\bar{u}s_u/u_s|$, $|u\bar{s}_s^2/\partial x| \gg |\bar{u}s_s\partial s/\partial x|$ and the role of $\bar{u}s_s\partial s/\partial x$ can be neglected. However, $|c_1q|$ can be large and entrainment fluxes may explain why a de-correlation exists between CO$_2$ and water vapor for dry soil moisture states. However, to derive rule-of-thumb guiding principle primarily informed by NDVI variability, the problem can be conceptually explored within the context of the time scale arguments of Belcher and Hunt (1998) using the 'disturbed boundary layer' analogy.

In Belcher and Hunt (1998), two time scales are proposed: (1) the advection–distortion time scale $T_{adv}$, which characterizes the time for turbulent eddies to be advected and distorted by the spatial mean gradients over some horizontal distance $L_a$ defining the length scale of inhomogeneity (e.g. here connected with the scalar source variations that induce longitudinal mean scalar gradients, etc.), and (2) the de-correlation or relaxation time scale of the large energy-containing eddies. For MOST, the relaxation time scale $\tau$ was shown to be the canonical time scale for the equilibrium between scalar variance production and its dissipation. Stated differently, in a stationary boundary layer and in the absence of subsidence, a balance between local scalar variance production and its dissipation is maintained if $T_{adv} \gg \tau$ so that the turbulence can come into local equilibrium with the surrounding mean scalar gradients (or the scalar fluxes producing them) before being advected. By contrast, the so-called 'rapid-distortion regions' occur when $T_{adv} \ll \tau$ and the mean flow advects turbulent eddies over $L_a$ more rapidly than they interact nonlinearly in their cascade towards dissipation.

Fig. 8 – Variations of $c_1s = \bar{u}s/\bar{u}s$ with $s$ being temperature, water vapor and CO$_2$ as function of atmospheric stability for the three hydrologic conditions.
Conceptually, when eddies are in contact with heterogeneous scalar sources (or sinks) at the ground, they must loose their coherency much more rapidly before advecting past the sensor location to recover M–O scaling. For the experimental setup here, we assume that $L_x = L_x$ and $T_{adv} = L_x/u_x$ at least for the purposes of a first order analysis aimed at constructing a rule-of-thumb (without regards to the stability class or entrainment cases earlier described).

Based on Belcher–Hunt argument, when $L_x \gg kz(\bar{u}/u_z)$ the relaxation time scale of turbulent eddies is too short for the mean flow to distort them thereby maintaining their equilibrium with the underlying surface. For these conditions, predictions by the FV method as well as M–O scaling should hold. The values of $kz(\bar{u}/u_z)$ did not change dramatically with shifts in hydrologic states and ecosystem composition. In fact, comparing the histograms of $\bar{u}/u_z$ for wet and dry periods (not shown), no appreciable difference was detected, with modal values ranging from 5 to 6. For wet conditions and with NDVI used as a surrogate measure of scalar source distribution, $L_x$ (~100 m) was much larger than $kz(\bar{u}/u_z)$ (~20 m); hence, agreement between MOST predictions (i.e. production balancing dissipation) and the data is consistent with the Belcher–Hunt argument (extended to scalars here). However, for dry conditions, $L_x$ (~10 m) is comparable to $kz(\bar{u}/u_z)$ suggesting that distortions by the mean flow can disrupt the balance between production and dissipation terms in Eq. (7). Hence, in a first order analysis, differences in $L_x$ between wet and dry states remain the determining factor for explaining differences in $T_{adv}$.

Furthermore, $\bar{u}/u_z (\sim 6) \gg \sqrt{\bar{u}^2}/u_z$. This supports the argument in Section 4.3 except for neutral cases, where the two terms may be comparable for water vapor. Also, note that the disturbed boundary layer analogy is recovered from the scaling arguments in Section 4.3 if TR is neglected relative to the production term and $\bar{u}/u_z \gg \sqrt{\bar{u}^2}/u_z$. Hence, the Belcher–Hunt disturbed boundary layer argument can be extended to the scalar variance budget analysis in Section 4.3 and is consistent with the data reported here. However, this argument must be viewed as a necessary but not sufficient condition for measurements to diverge from M–O scaling predictions for FV functions. Intrinsic in the extension of the Belcher–Hunt argument to scalar variances is the assumption that $\bar{u} \partial \bar{u}^2/\partial x \gg |TR|$, which we showed is not likely for the dry soil moisture states. In other words, for heterogeneous source–sink distribution in which the convective boundary layer is dry and deep, both $\bar{u} \partial \bar{u}^2/\partial x$ and $|TR|$ may be impacting FV predictions. It is for this reason that we frame the advection–distortion argument as a necessary but not sufficient condition for the application of MOST to FV analysis.

6. Summary and conclusions

How land-cover heterogeneity (LCH) in NDVI impacts M–O scaling for three scalars temperature, water vapor, and carbon dioxide were explored. When grass and trees dominate the landscape (wet soil moisture states), M–O scaling was recovered. However, when bare soil and trees dominate the landscape, large departures from M–O scaling were measured. Among the three scalars, water vapor was the least compatible to M–O scaling (when compared to temperature), which was surprising given the similarity in sources and sinks between CO2 and water vapor at the ground. To explain this anomalous behavior, a number of scaling arguments and analyses were performed. The dependence of $\psi_{1q}$ on $\zeta$ appears to be much higher than $\psi_{1c}$ irrespective of the soil moisture state. This finding partially explains why $\psi_{1q} > \psi_{1c}$. The correlation analysis between $q$ and $\zeta$ for the dry convective boundary layer hints that entrainment from the capping inversion, along with other modulations from the outer layer, can be responsible for the different behavior of the two scalars. To explain how LCH in NDVI affected the FV predictions, we extended the disturbed boundary layer analogy of Belcher and Hunt (1998) to include scalar source heterogeneity. An integral length scale $L_x$, estimated from the integrated 2-D autocorrelation of the NDVI, was assumed to represent the coherence of the disturbances impacting horizontal gradients. When $L_x \gg kz(\bar{u}/u_z)$, M–O scaling was recovered. However, when $L_x \sim kz(\bar{u}/u_z)$, a significant departure between MOST predictions and measurements were found, especially for water vapor and CO2. The length scale argument developed here was based on two canonical time scales representing disturbed boundary layers: the advection–distortion and the relaxation time scale. We emphasized that this length scale argument is a necessary but not sufficient condition because both $\bar{u} \partial \bar{u}^2/\partial x$ and $|TR|$ can impact FV predictions.

Appendix A. Orientation of the eddy-covariance sensor in complex terrain

In a coordinate system $(x, y, z)$, the three velocity components are defined as $u$, $v$ and $w$. Over a sloping planar surface, the velocity components $u$ and $w$ should be taken parallel and normal to this surface, respectively. If the axis of the sonic anemometer is not orientated parallel to this surface then a fraction of the horizontal velocity is recorded as vertical velocity (with significant implications to scalar fluxes).

When measuring flow statistics in complex terrain, a displaced coordinate system is preferred because this system reduces to terrain following near the ground and rectangular well above the surface. The effective slope sensed by the sonic anemometer at some height, often referred to as pitch angle, varies with topography, and hence, with the wind direction. Two approaches can be followed to perform the correction: (1) a short term rotation applied for each time-averaging period so that $w = 0$ and (2) a long-term ensemble-averaged-rotation such as the pitch angle (i.e. $\arctg(\bar{w}/\bar{u})$) is evaluated for every direction from an ensemble of sufficiently large data series.

The relevant flow statistics in the transformed coordinates can be derived from the original statistics (shown in capital letters for clarity) in the sonic anemometer coordinate system $(X, Y, Z)$ using a rotation matrix. This matrix can be obtained by applying two consecutive rotations, the first along the Z-axis of an angle $\alpha = \arctg(V/U)$ to align the x-axis to the mean flow direction so $\theta = 0$ (azimuthal rotation). The second rotation is along the crosswind axis of an angle $\phi$.
equal to the pitch (zenithal rotation). In three dimensions, a rotation can be defined by three Euler angles or by a single angle of rotation and the direction of a vector about which to rotate. In the latter case the matrices required to rotate a column vector in Cartesian coordinates about the origin are given by:

\[
A_z = \begin{pmatrix}
\cos \alpha & \sin \alpha & 0 \\
-\sin \alpha & \cos \alpha & 0 \\
0 & 0 & 1
\end{pmatrix}
\]

along the Z-axis, and

\[
A_z = \begin{pmatrix}
\cos \phi & 0 & -\sin \phi \\
0 & 1 & 0 \\
\sin \phi & 0 & \cos \phi
\end{pmatrix}
\]

along the y-axis.

The rotation matrix \( R(\alpha, \phi) \) is evaluated as the product \( R = A_z \times A_x \), where \( \times \) is a matrix multiplication operator.

To reconstruct all the wind and scalar statistics in the new coordinate system, we use matrix notation and define \( u_\perp = [\bar{u} \bar{v} \bar{w}]^T \) and \( U_\perp = [\bar{U} \bar{V} \bar{W}]^T \). With these definitions, the mean velocity components will be:

\[
\bar{u} = R^T U = R \times U
\]

All the second-order statistics, which are represented by the variance-covariance matrix

\[
cov = \left(\begin{array}{ccc}
\bar{u}^2 & \bar{u}\bar{v} & \bar{u}\bar{w} \\
\bar{u}\bar{v} & \bar{v}^2 & \bar{v}\bar{w} \\
\bar{u}\bar{w} & \bar{v}\bar{w} & \bar{w}^2
\end{array}\right)
\]

and

\[
COV = \left(\begin{array}{ccc}
\bar{U}^2 & \bar{U}\bar{V} & \bar{U}\bar{W} \\
\bar{U}\bar{V} & \bar{V}^2 & \bar{V}\bar{W} \\
\bar{U}\bar{W} & \bar{V}\bar{W} & \bar{W}^2
\end{array}\right)
\]

are evaluated as follow:

\[
cov = \left(\bar{u} - \bar{u}_\perp\right) \times \left(\bar{u} - \bar{u}_\perp\right)^T = R^T (U - \bar{U}_\perp) \times (U - \bar{U}_\perp)^T = R \times (U - \bar{U}_\perp) \times (U - \bar{U}_\perp)^T = R \times COV \times R^T
\]

Similarly, for the scalar turbulent fluxes expressed as

\[
f_{\perp c} = \left[\bar{u}c \bar{V}c \bar{W}c\right]^T \quad \text{and} \quad f_{\perp c} = \left[\bar{U}c \bar{V}c \bar{W}c\right]^T
\]

as discussed by Detto and Katul (2007) is presented. Removing the density fluctuations induced by external temperature and humidity fluctuations \( (\rho_{ext}) \) from the measured density fluctuations \( \rho_c \) results in a ‘natural’ scalar density fluctuation \( \rho_{c,nat} \) given by

\[
\rho_{c,nat} = \rho_c - (\rho_{ext}) = \rho_c - \left( \frac{\rho_c}{\rho_0} \rho_0^* + \bar{\mu}(1 + \mu\sigma) \frac{\bar{T}}{T} \right)
\]

where \( \mu \) is the ratio of molecular mass of dry air to water vapor, \( \bar{\mu} = \rho_c/\rho_0 \) (Detto and Katul, 2007), and \( \rho_{ext} = 0 \). Note that \( \rho_{ext} \) is a scalar quantity and thus independent of any coordinate rotation. Detto and Katul (2007) showed that the concomitant fluxes and variances can be expressed as

\[
\bar{u}_\parallel \rho_{c,nat}^\prime = \bar{u}_\parallel \rho_{c} + \frac{\mu}{\rho_0} \rho_0^* \rho_0^\prime + \rho_0(1 + \mu\sigma) \frac{u_T^2}{T}
\]

where \( \bar{u}_\parallel = (u', v', w') \) are the turbulent velocity fluctuations in direction \( k_{\parallel} = (x, y, z) \) with \( x \) being the longitudinal, \( y \) being the lateral, and \( z \) being the vertical coordinates, respectively, and

\[
\bar{v}_{\parallel} \left( \frac{\bar{T}}{T} \right) \rho_{c,nat}^\prime = \bar{v}_{\parallel} \rho_{c} + \mu \frac{\rho_c}{\rho_0} \rho_0^* \rho_0^\prime + \rho_0(1 + \mu\sigma) \frac{v_T^2}{T} + \rho_0(1 + \mu\sigma) \rho_T \frac{v_T^2}{T} + \rho_0(1 + \mu\sigma) \rho_T \frac{v_T^2}{T}
\]

The covariance between two scalars \( \rho_{c1,nat} \rho_{c2,nat} \) is also given by

\[
\bar{v}_{\parallel} \rho_{c1,nat} \rho_{c2,nat} = \rho_{c1,nat} \rho_{c2,nat} + \frac{\mu}{\rho_0} \left( \rho_{c1,nat} \rho_0^* \rho_0^\prime + \rho_{c1,nat} \rho_0(1 + \mu\sigma) \frac{u_T^2}{T} \right)
\]

All terms that appear on the right-hand side of equations (B1)–(B5) are variances or covariances that can be independently measured by infrared gas analyzers and sonic anemometers. For flat terrain and for \( i = 3 \), the standard WPL correction (Webb et al., 1980) is recovered from B1.

The importance of these adjustments were demonstrated at a grass-covered forest clearing experiment conducted at the Duke Forest, near Durham, North Carolina using 10 Hz measurements of \( \mathrm{CO}_2 \), water vapor, and temperature (see Detto and Katul, 2007).

**Appendix B. Simplified expressions for adjusting second-order statistics of scalar density measurements**

A summary of the corrections to scalar variances, horizontal and lateral turbulent fluxes, and covariance between the temperature and other tracers as well as the covariance amongst two tracers measured by an open-path gas analyzer


