The non-local character of turbulence asymmetry in the convective atmospheric boundary layer

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The inadequacy of conventional gradient diffusion in closure modelling of turbulent heat fluxes within the convective atmospheric boundary layer is often alleviated by accounting for non-local transport effects, such as Deardorff’s counter-gradient models, Wyngaard’s transport asymmetry closures or mass-flux parametrization. This concept of large-eddy flux transport is examined here with the principal aim of unifying these seemingly different models. Using large-eddy simulation (LES) runs for the atmospheric boundary layer, spanning weakly to strongly convective conditions, a generic diagnostic framework that encodes the role of third-order moments in non-local transport is developed and tested. The premise is that these non-local effects are responsible for the inherent asymmetry in vertical transport and hence the necessary non-Gaussian nature of the joint probability density function (JPDF) of vertical velocity and potential temperature must account for these effects. Conditional sampling (quadrant analysis) of this JPDF and the imbalance between the flow mechanisms of ejections and sweeps are used to characterize this asymmetry, which is then linked to the third-order moments using a cumulant-discard method for the Gram–Charlier expansion of the JPDF. While the concept of ejection-sweep events used here is not a simple extension of that commonly used in the surface layer, their connection to third-order moments shows that the concepts of bottom-up/top-down diffusion or updraught/downdraught models are accounted for by various quadrants of the JPDF. An analogy between mass-flux models and the relaxed eddy accumulation method reveals that there is a seemingly implicit assumption of a Gaussian JPDF in the former.

Key Words: convective boundary layer; quadrant analysis; ejection-sweep events; heat flux; second-order closure; turbulence asymmetry

Received 27 May 2016; Revised 4 October 2016; Accepted 6 October 2016; Published online in Wiley Online Library 1 December 2016

1. Introduction

Despite their introduction some 140 years ago by Boussinesq, eddy diffusivity and eddy viscosity (or simply K-theory) models remain key concepts in turbulence research. According to McComb (2004), they qualify as the first successful application of renormalization group (RNG) methods, well before RNG’s formal development in quantum field theory. The use of K-theory has made it possible to estimate and model turbulent fluxes in natural systems operating at Reynolds numbers that are simply too large to resolve in direct numerical simulations. However, the failure of K-theory in the convective atmospheric boundary layer (CABL) continues to draw research interest for an alternative that retains its simplicity. The CABL is a common daytime occurrence over the land surface and is characterized primarily by ascending buoyant plumes that originate at the heated surface and evolve to a length-scale comparable to the boundary-layer depth h. These semi-organized eddies are accompanied by weaker subsiding (descending) plumes associated with entrainment fluxes at the boundary-layer top, leading to an asymmetry in the turbulence structure and hence in the vertical transport of scalars (e.g. heat, humidity) within the CABL. This perspective of a global boundary layer consisting of large-scale updraughts (bottom-up) and downdraughts (top-down) is now known to be the principal flux-transport mechanism of heat in the well-mixed layer. Often referred to as non-local transport, as opposed to local mean gradient-diffusion closures (K-theory) driven by mean scalar gradients, a variety of modelling approaches have emerged over the past decades to explain and model the effects of these non-local large eddies on turbulent fluxes. The tenets of such models...
descend from different schools of thought in the atmospheric boundary-layer literature and, apart from minor advantages of each model over the others in certain situations, they involve some commonalities and invariably have comparable performance. This begs the question as to whether there is a unifying ‘umbrella’ framework that encodes the mechanisms of vertical transport of scalars in the CABL, attributes the differences among the available models to derivatives of some parent process and lends itself to a wider variety of applications requiring more efficient parametrization of boundary-layer processes.

In that respect, the vertical transport of heat in the clear-air (dry), horizontally homogeneous, quasi-stationary, convective atmospheric boundary layer is considered here. This setting has a long history in the pedagogy of atmospheric boundary-layer turbulence and was considered in the early works of Ertel (1942), Priestley and Swinbank (1947), Deardorff (1966) and Zeman and Lumley (1976) on failures of K-theory. It was evident that, in the well-mixed portion of a convective boundary layer, finite heat fluxes coexist with negligible vertical gradients in the corresponding mean potential temperature (often referred to as ‘zero-gradient’ flow). The local eddy-diffusivity approach was therefore insufficient to explain such fluxes in sign and magnitude. The latter approach (K-theory) assumes that the vertical flux of a turbulent scalar quantity, such as potential temperature $\theta$, is proportional to the gradient in its local mean value ($\overline{\theta}$) using a turbulent heat diffusivity $K_{\theta}$, such that (e.g. Stull, 1988)

$$\overline{\theta'} = -K_{\theta} \frac{d\overline{\theta}}{dz},$$

where $\theta'$ is the turbulent fluctuation in the vertical velocity component and $z$ is the vertical coordinate. Henceforth, small letters represent instantaneous turbulent fluctuations in a variable, capital letters are reserved for mean quantities and overbars represent averaging over coordinates of statistical homogeneity (time and planar space here). Figure 1 is a sample result from a large-eddy simulation (LES) run described in later sections that illustrates the limitation of K-theory in CABL, where $d\overline{\theta}/dz = 0$ yet $\overline{\theta'} > 0$. In fact, the upper part of the CABL experiences both positive gradients and fluxes, which reflects the ability of buoyancy-driven plumes to transport warm air from the surface to the top of the boundary layer and hence ascend counter to the gradient in mean potential temperature (e.g. Deardorff, 1972; Wyngaard and Weil, 1991). This observation initiated interest in non-local large-eddy flux transport as a means to correct for K-theory and improve the parametrization of the CABL in regional and general circulation models.

While there is a significant body of literature and reviews on this topic (e.g. Zilitinkevich et al., 1999; van Dop and Verver, 2001), a brief summary of the common modelling approaches correcting for non-local effects is presented here.

(i) **Eddy diffusivity–counter-gradient (EDCG).**

The premise of this approach is the addition of a counter-gradient term ($\gamma$) to Eq. (1) (Deardorff, 1972; Troen and Mahrt, 1986; Holtslag and Moeng, 1991; Holtslag and Boville, 1993):

$$\overline{\theta'} = -K_{\theta} \frac{d\overline{\theta}}{dz} - \gamma,$$

such that the term $K_{\theta}\gamma = \overline{\theta'}_{NL}$ represents the non-local (NL) component of the heat flux. Deardorff (1972) initially suggested

$$\gamma = \beta \frac{\sigma_{\theta}^2}{\sigma_{\overline{w}}^2},$$

where $\beta = g/T_0$ is the buoyancy parameter, $g$ is the gravitational acceleration, $T_0$ is a reference absolute temperature and $\sigma_{\theta}^2 = \overline{\theta'^2}$ and $\sigma_{\overline{w}}^2 = \overline{w'^2}$ are the variances in potential temperature and vertical velocity, respectively. A limitation to Eq. (3) is the fact that $\sigma_{\theta}^2$ and $\sigma_{\overline{w}}^2$ can...
be large and even comparable to the gradient-diffusion term in the atmospheric surface layer, where K-theory is expected to hold. Improved parametrization appeared in the works of Troen and Mahrt (1986) and Holtslag and Moeng (1991), where the former proposed an expression for \( \gamma \) to be compatible with surface-layer similarity theory, resulting in

\[
\gamma = C \frac{\overline{w^3}}{w_s h},
\]

where \( C \) is a proportionality constant, \( \overline{w^3} \) is the kinematic surface heat flux, \( h \) is the boundary-layer height, \( w_s \approx 0.65v_w \) (convective limit) is a mixed-layer velocity scale and \( w_s = (\beta \overline{w^3} h) / \beta \) is known as Deardorff’s convective velocity scale (Deardorff, 1970). With a simple parametrization of the gradient in the third-order moment \( \overline{w^3} \), based on the LES results of Moeng and Wyngaard (1989), Holtslag and Moeng (1991) expressed the counter-gradient correction as

\[
\gamma \propto \frac{w_s \overline{w^3}}{\sigma_\theta^2 h},
\]

depending on the effects of the bulk parameters \( (w_s, h \text{ and } \overline{w^3}) \) of the CABL in the heat-flux profile. In this EDCG framework, the height-dependent turbulent heat diffusivity is considered proportional to the vertical velocity variance and an appropriate time-scale \( (K_H \propto \tau^2) \), analogous to Taylor diffusion (Taylor, 1922). Nevertheless, rather than a Lagrangian time-scale as in Taylor’s original work (Taylor, 1922), \( \tau \) here is associated with Rotta’s return-to-isotropy time-scale (Deardorff, 1972) or the mean turbulence kinetic energy (TKE) dissipation rate (Holtslag and Moeng, 1991).

(ii) **Transport asymmetry (TA).**

In a remarkable series of articles, Moeng and Wyngaard (1984, 1989), Wyngaard and Brost (1984), Wyngaard and Weil (1991) and Wyngaard and Moeng (1992) introduced and formulated the concept of asymmetry in the vertical diffusion of scalars in the CABL. In particular, they distinguished bottom-up diffusion (driven mostly by surface flux) from top-down (driven by entrainment flux), noting that these mechanisms have different profiles of scalars in the CABL. In particular, \( \gamma \) introduced and formulated the concept of asymmetry in the vertical transport, which is in turn associated with the TOM \( (\overline{w^3}) \). This hints at the importance of the non-Gaussian nature of the turbulence structure in the CABL as a means to explain the non-local heat transport, which is responsible for non-local transport in the CABL. The TOM calls attention to their parametrization. The TOM are often obtained by solving the corresponding budget equations involving fourth-order moments (FOM) with the quasi-normal decomposition (Canuto et al., 1994) or mass-flux decomposition of the higher-order terms (e.g. Abdella and McFarlane, 1997; Grynavik and Hartmann, 2002). Examples of such parametrizations are (Abdella and McFarlane, 1997)

\[
\overline{w^3} = C_{w^3} \overline{w^3} \sigma_\theta^2,
\]

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\]

Mironov et al. (1999) proposed that the skewness of potential temperature \( (\overline{\theta}) \) should replace \( \overline{w^3} \) in Eq. (8).

(iv) **Eddy diffusivity–mass flux (EDMF).**

This model parametrizes the turbulent flux in the CABL on the basis of separating the boundary layer into strong and narrow updraughts and a surrounding turbulent environment. The formulation of this method was initially developed for convective transport in cumulus clouds and was later extended to the full boundary layer (Siebesma and Cuijpers, 1995; Siebesma and Teixeira, 2000; Siebesma et al., 2007). The total turbulent flux of potential temperature is then due to the contributions from the updraughts, the surrounding environment and a mass-flux term:

\[
\overline{w^3} = a_u \overline{w^3} u + (1 - a_u) \overline{w^3} e + a_u (w_u - \overline{w})(\theta_u - \overline{\theta}),
\]

where the sub- or superscripts ‘u’ and ‘e’ denote strong updraughts and the surrounding environment, respectively, \( a_u \) is the fractional area occupied by the updraughts, \( w_u \) and \( \overline{w} \) are the mean vertical velocity components in the updraught and the complementary environment and \( \overline{\theta} \) and \( \overline{\theta} \) are the corresponding mean potential temperatures. Neglecting the first term in Eq. (9) \( (a_u \ll 1) \) and with the approximation \( \overline{\theta} = \overline{\theta} \), the EDMF model is usually reduced to

\[
\overline{w^3} = -K_H \frac{d\overline{\theta}}{dz} + M(\overline{\theta} - \overline{\theta}),
\]

where \( \overline{w^3} = -K_H \frac{d\overline{\theta}}{dz} \) represents the eddy-diffusivity term and \( M = a_u (w_u - \overline{w})(\overline{\theta} - \overline{\theta}) \) defines the convective mass flux. The second term in Eq. (10) is equivalent to the non-local heat flux \( \overline{w^3} \) and requires parametrization of the mass flux \( M \) and an updraught model for \( w_u \) and \( \overline{\theta} \), besides the eddy diffusivity \( K_H \).

Notwithstanding the differences across the models described above, it is evident in all cases that the large-eddy coherent motion in the CABL primarily dictates the vertical diffusion of scalars. It is also apparent that the non-local fluxes are a manifestation of the inherent asymmetry in vertical transport, which is in turn associated with the TOM \( (\overline{w^3}) \) and their vertical gradients. This hints at the importance of the non-Gaussian nature of the turbulence structure in the CABL as a means to explain the non-local transport, where such asymmetry must exhibit itself in the joint probability density function (JPDF) of vertical velocity and potential temperature. While the latter argument is only intuitive, this JPDF has received little attention in the context of non-local scalar flux literature, except for the work of Wyngaard and Moeng (1992) and Sullivan et al. (1998), which provided a reasonable starting point for the work here.

The second-moment budget of the sensible heat flux in the weakly-to-strongly convective atmospheric boundary layer is considered here to explore the role and relative importance
of the TOM on non-local flux transport. The premise is that the non-Gaussian JPDF of vertical velocity and potential temperature encodes all the properties of these TOM and hence provides a unifying framework to explain all the underlying physical mechanisms of non-local flux corrections to K-theory. Since the essence of second-order closure modelling is the proper parametrization of the TOM, the aforementioned models (EDCG, TA, TOMP and EDMF) seem to be a natural extension to the characteristics of this JPDF. Although the intent here is not to provide a fully prognostic closure replacing earlier models for flux parametrization, we build on the works of Nakagawa and Nezu (1977) and Raupach (1981) on conditional sampling (quadrant analysis) and the cumulant-discard expansion of the Gram–Charlier JPDF of \( w \) and \( \theta \) to unfold dynamically interesting connections between EDCG, TA, TOMP and EDMF models and the ejection–sweep events in the flow field. While the aforementioned work examined the fractional contributions of each quadrant to the Reynolds stresses (momentum fluxes), the analysis can be extended to scalar fluxes (\( \overline{w\theta} \)) (Katul et al., 1997; Cava et al., 2006; Poggi and Katul, 2007). It is to be noted, however, that the use of the terms ‘ejections’ and ‘sweeps’ here is not a simple mapping of what is commonly understood in the context of momentum fluxes in the surface layer (i.e. ejection–sweep cycle). Rather, an analogy of the notation used by Raupach (1981) with quadrant analysis of the heat flux is made for convenience of notation and the term ejection/sweep ‘events’ is used throughout in lieu of ‘cycle’. This point is revisited in section 2.3 when introducing the nomenclature for quadrant analysis. Most importantly, conditional sampling of the \( \overline{w\theta} \) JPDF quantifies the fractional contributions of each quadrant to the total heat flux and ties these contributions to physical characteristics of the flow field, namely the ejections, sweeps, inward and outward interactions. Connections between these flow mechanisms and the TOM then provide a gateway to explain their relative roles in non-local transport and their representation in models such as EDCG, TA, TOMP and EDMF. The analysis uses a suite of LES experiments to provide the required profiles of all moments up to third order to complement the work and, in the interest of completeness, the article also examines the performance of various closure time/length-scales and turbulent diffusivity profiles.

2. Theory

As noted earlier, the CABL considered here is clear-air, stationary (\( \partial \Phi/\partial t = 0 \)), planar homogeneous \( \partial \Phi/\partial x = \partial \Phi/\partial y = 0 \), with high Reynolds and Peclet numbers (negligible molecular viscosity) and negligible Coriolis force. The coordinate system is defined such that \( x, y, \) and \( z \) form the longitudinal, lateral and vertical directions, respectively. The usual Reynolds decomposition notation is employed throughout, where all variables are decomposed into stationary mean (capital letters) and fluctuating (small letters) quantities. In this section, the characteristics of the heat-flux budget with various simplifying closure assumptions are presented. These assumptions are then tested and discussed in section 4.

2.1. The heat-flux budget

Using the aforementioned simplifying conditions and adopting the Boussinesq approximation, the heat-flux budget in the convective boundary layer reduces to

\[
\frac{\partial \overline{w\theta}}{\partial t} = 0 = -\sigma_{\theta}^w \frac{d\theta}{dz} - \frac{\partial \overline{w\theta}}{\partial x} - \frac{1}{\rho_0} \frac{\partial p}{\partial z} + \beta \theta^2, \tag{11}
\]

where \( \rho_0 \) is a reference-state air density and \( p \) is the pressure fluctuation referenced to the hydrostatic state and its finite value is attributed to turbulence. The flux production/destruction terms on the right-hand side (rhs) of Eq. (11) are, respectively, the mean-gradient production (\( M \)), the turbulent flux transport (\( T \)), the pressure gradient--potential temperature covariance (\( P \)) and the buoyancy production (\( B \)). The term \( P \) acts as a destruction/sink term for the heat flux \( \overline{w\theta} \) and, following Rotta (1951), who initially proposed the return-to-isotropy parametrization for the pressure–velocity gradient covariance in turbulent shear flows, numerous studies have extended this parametrization to incorporate the contributions from the mean-gradient, buoyancy and Coriolis effects (Jones and Musonge, 1984; Moeng and Wyngaard, 1986; Andrén and Moeng, 1993; Mironov, 2001). Since the Coriolis force is neglected here, the general form of the parametrization of \( P \) is

\[
P = -\frac{1}{\rho_0} \frac{\partial \theta}{\partial z} = -C_{1w} \overline{w\theta} - C_2 \beta \theta^2 + C_3 \sigma_{\theta}^w \frac{d\theta}{dz}, \tag{12}
\]

where the first term on the rhs represents Rotta’s return-to-isotropy (slow) part and is inversely proportional to a relaxation time-scale \( \tau_1 \), and the last two terms are referred to as the rapid part. Typical values of the constants are \( C_1 = 3 \), \( C_2 = 1/3\)-1/2 and \( C_3 = 2/5 \). The performance of the parametrization in Eq. (12) with different relaxation time-scales will be evaluated with LES simulations in section 4. Using Eq. (12) and maintaining the constants for the time being, the flux budget Eq. (11) can be written as

\[
\overline{w\theta} = C_1 - \frac{1}{\tau_1} \sigma_{\theta}^w \frac{d\theta}{dz} - \frac{1}{(C_3 - 1)\sigma_{\theta}^w} \frac{\partial \overline{w\theta}}{\partial x} + \frac{1 - C_2}{(C_3 - 1)\sigma_{\theta}^w} \beta \theta^2, \tag{13}
\]

where, again, \( C_1 < 1 \); it has been predicted to be 2/5 for isotropic turbulence using rapid distortion theory, as discussed in Pope (2000). Equation (13) defines a general framework for the heat flux within the convective boundary layer and is analogous to the form of Eq. (2) that corrects for counter-gradient fluxes, with a diffusivity \( K_{\theta\theta} \propto \tau_1 \sigma_{\theta}^w \).

The first term on the rhs of Eq. (13) is responsible for the local flux and the last two terms are the origin of non-local fluxes. The ratio of variances term \( \propto \sigma_{\theta}^w/\sigma_{\theta}^w \) resulting from buoyant production is the counter-gradient correction obtained by Deardoff (1972) after ignoring the flux-transport term, while Holsgog and Moeng (1991) parametrized the latter with \( w_{\theta} \) and \( \overline{w\theta} \theta \) and assumed that the pressure gradient–temperature covariance cancels the buoyancy effects. The implicit assumption that the same diffusivity is applicable to local and non-local terms is debatable (e.g. Frech and Mahrt, 1995) and renders the choice of return-to-isotropy time-scale (\( \tau_1 \)) elusive. A local time-scale such as \( \tau_1 \propto TKE/\epsilon \), where \( \epsilon \) is the TKE dissipation rate, may not be characteristic of non-local fluxes, whereas a large-eddy turnover time-scale such as \( \tau_1 \propto h/w_{\theta} \) is not adequate for localized eddies.

By analogy with Eq. (2), the counter-gradient term reads

\[
\gamma = \frac{1}{(C_3 - 1)\sigma_{\theta}^w} \frac{\partial \overline{w\theta}}{\partial x} - \frac{1 - C_2}{(C_3 - 1)\sigma_{\theta}^w} \beta \theta^2. \tag{14}
\]

The contribution of each of these two terms, in both magnitude and sign (source/sink), will be discussed later. Equation (14) highlights the importance and the requirement of closure assumptions for the turbulent flux-transport term in the context of non-local fluxes.

2.2. Local closure to turbulent flux transport

The most common closure for the turbulent transport of scalar fluxes is again down-gradient diffusion. The rationale is that, while the gradient in first-order moments is small in the well-mixed...
layer and hence Eq. (1) is insufficient, the approach can be valid for the non-vanishing gradients in turbulent second-order moments. This can be attributed to the fact that equilibration between such turbulent quantities and their gradient is attained much faster than equilibration between mean gradient and turbulent quantities. This closure results in the conventional form

\[ \frac{d\bar{w}\theta}{dz} = -\frac{d}{dz} \left( \tau_1 q \frac{d\bar{w}\theta}{dz} \right), \tag{15} \]

where \( \tau_1 \) and \( q \) are time and velocity scales, respectively. The diffusivity here (\( K_\theta = \tau_1 q^2 \)) is not necessarily identical to \( K_{11} = \tau_1 \sigma^2_\theta \) and, using Eq. (15), the heat-flux budget in Eq. (13) can be written as a second-order ordinary differential equation:

\[ K_{11} \frac{d^2 \bar{w}\theta}{dz^2} + \left( \frac{dK_{11}}{dz} \right) \frac{d\bar{w}\theta}{dz} - C_1 \frac{\bar{w}\theta}{\tau_1} + (C_3 - 1) \sigma^2_\theta \frac{d\theta}{dz} + (1 - C_2) \beta^2 \theta^2 = 0. \tag{16} \]

For a turbulent heat flux that is linear in \( z \), a negligible mean gradient term (\( \propto d\theta/dz \)) and a constant \( K_1 \), Eq. (16) reduces to

\[ \frac{\bar{w}\theta}{\tau_1} = 1 - \frac{C_2}{C_1} \theta \beta^2, \tag{17} \]

which implies that \( \tau_1 < 0 \) near the top of the CABL (where \( \bar{w}\theta < 0 \)). It also requires that the quantity \( \tau_1 \beta^2 \) be linear in \( z \). Including the mean gradient term retrieves the model by Deardorff (1972) shown earlier in Eq. (3) and hence it follows that \( K_1 \) must not be constant.

### 2.3. Conditional sampling and ejection-sweep events

To characterize the total heat flux \( \bar{w}\theta \) at a given height \( z \) in the CABL as the sum of contributions from different physical mechanisms, the JPDF of vertical velocity and potential temperature fluctuations, denoted by \( f(w, \theta) \), and the conditional sampling of its four quadrants are considered. Such sampling methods were reviewed in Wallace et al. (1972), Antonia (1981) and Bogard and Tiederman (1987). In analogy with momentum transport, four quadrants defined by the Cartesian axes of the scatter plot of \( w \) and \( \theta \) are shown in Figure 2. Quadrants I (\( w > 0, \theta > 0 \)) and III (\( w < 0, \theta < 0 \)) contribute to positive heat fluxes, but due to different physical mechanisms, namely warm air parcels moving upward and cold air parcels sinking, respectively. When the total heat flux \( \bar{w}\theta \) is positive, which is the case for roughly the lower 80% of the CABL (see Figure 1), quadrants I and III have a dominant contribution and are defined here as ejections and sweeps. While the terms ‘ejections’ and ‘sweeps’ are usually reserved for momentum fluxes, we adopt them here for heat fluxes with proper handling of the sign of the flux itself. Quadrants II (\( w < 0, \theta > 0 \)) and IV (\( w > 0, \theta < 0 \)) both contribute to negative fluxes associated with sinking warm air and rising cold air, respectively. The latter quadrants dominate in the top ≈ 20% of the CABL, when the total heat flux is negative due to entrainment from the free troposphere, and therefore events in these two quadrants are labelled as ejections and sweeps in this context. Additionally, ejections/sweeps as defined here are not analogous to updraughts/downdraughts used in the context of mass-flux models. The latter are defined by conditioning on the vertical velocity fluctuations only, i.e. updraughts correspond to \( w \) being positive (or larger than some threshold) and downdraughts correspond to \( w < 0 \). In the quadrant analysis here, updraughts would then be reflected in quadrants I and IV (both with \( w > 0 \)) and hence can contribute to positive heat fluxes (quadrant I) by carrying positive temperature fluctuations upward and negative heat fluxes (quadrant IV) by carrying negative temperature fluctuations upward. A similar picture follows for downdraughts reflected in quadrants II and III. On the other hand, ejection and sweep events are hereafter limited to quadrants I and III; respectively (or quadrants II and IV in the entrainment zone, where the net heat flux is negative). This is the main physical difference between ejections and updraughts or sweeps and downdraughts.

For stationary flow in the CABL, the contribution to the total heat flux from quadrant \( i \) can be written as (Raupach, 1981)

\[ \langle w\theta \rangle_i = \frac{1}{T_p} \int_0^{T_p} w(t) \theta(t) I_i \, dt, \tag{18} \]

where the angled brackets denote conditional averaging, \( T_p \) is the averaging time period and the indicator function \( I_i \) is defined such that

\[ I_i = \begin{cases} 1 & \text{if the events (\( w, \theta \)) both occur in quadrant } i, \\ 0 & \text{otherwise,} \\ \text{where } i = I, II, III, IV. \end{cases} \tag{19} \]

The fraction of heat flux contributed by quadrant \( i \) is then given by

\[ F_i = \frac{\langle w\theta \rangle_i}{\bar{w}\theta}, \tag{20} \]

implying that, in the upward (positive) heat-flux portion of the CABL, \( F_i > 0 \) when \( i \) is odd (ejections and sweeps) and \( F_i < 0 \) otherwise, with \( F_1 + F_2 + F_3 + F_4 = 1 \). The opposite occurs close to the entrainment zone, where the heat flux is downward, i.e. \( F_i > 0 \) when \( i \) is even. It also follows that these fractional contributions are related to the JPDF by

\[ F_i = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} w\theta f(w, \theta) I_i \, dw \, d\theta, \tag{21} \]

and, since \( f(w, \theta) \) can be specified in terms of its moments (ideally infinite set), Eq. (21) provides a link between the fractional contributions of heat fluxes from each quadrant to the total heat flux. For such a quadrant representation, the interest here is in the balance between the contributions of rising warm air (quadrant I ≡ ejections) and sinking cold air (quadrant III ≡ sweeps) to the positive heat

Figure 2. Nomenclature for conditional sampling of the \( w-\theta \) events. Quadrants I and III contribute to positive (upward) heat fluxes, while quadrants II and IV contribute to negative (downward) fluxes. In the region where the net heat flux is positive (lower ≈ 80% of the CABL), quadrants I and III are defined here as ejection and sweep events, respectively. Quadrants II and IV correspond to ejection and sweep events in the negative net heat flux region (upper ≈ 20% of the CABL).
Adams–Bashforth method is used for time advancement. The form. Spatial derivatives are discretized through second-order between different flow features in contributing to the total heat flux, Eq. (23) encompasses the role of each TOM in shaping the above incorporate some TOM in representing the non-local heat flux, or otherwise the imbalance between quadrants II and IV in contributing to the negative heat flux. This imbalance reflects the relative importance of each of these mechanisms and can be quantified as

\[
\Delta F = \frac{1}{R\sqrt{2\pi}} R \left( M_{03} - M_{00} \right) + \frac{1}{2} \left( M_{21} - M_{12} \right),
\]

where \( R = \overline{w\theta}/\sigma_w\sigma_\theta \) is the correlation coefficient and the moments \( M_k \) are defined by

\[
M_k = \frac{\overline{w^k\theta}}{\sigma_w^k\sigma_\theta^k}.
\]

Hence \( M_{03} = \overline{w^3\theta}/\sigma_v^3 \) and \( M_{10} = \overline{w\theta}/\sigma_w^3 \) define the skewness of the vertical velocity component and potential temperature, respectively, while \( M_{21} = \overline{w^2\theta}/\sigma_w^2\sigma_\theta \) and \( M_{12} = \overline{w\theta}/\sigma_w^2\sigma_\theta \) are the central mixed-moment representations of the flux of potential temperature variance and flux of heat, respectively. Equation (23) was derived for momentum transport in the atmospheric boundary layer, where \( \overline{w\theta} < 0 \), and hence it similarly applies to \( \Delta F = \overline{F IV} - \overline{F I} \) in the context of heat flux transport. Nonetheless, it can be adapted to the positive heat-flux case \( \Delta F = \overline{F IV} - \overline{F I} \) simply by switching the sign of \( w \) in the terms where it occurs an odd number of times. While the various models introduced above incorporate some TOM in representing the non-local heat flux, Eq. (23) encompasses the role of each TOM in shaping the asymmetry in \( J(w, \theta) \) and connects this role to the imbalance between different flow features in contributing to the total heat flux in the CABL.

3. LES runs

The LES code used here solves the three-dimensional filtered equations for momentum and temperature written in rotational form. Spatial derivatives are discretized through second-order centred finite differences in the vertical and pseudospectral differentiation in the horizontal directions. The second-order Adams–Bashforth method is used for time advancement. The details of the LES code, the numerical scheme used, the grid generation and sub-grid-scale (SGS) modelling and post-processing of LES output can be found in Kumar et al. (2006) and Salesky et al. (2016). The SGS model used is the Lagrangian-averaged scale-dependent dynamic model (Bou-Zeid et al., 2005), which applies the dynamic procedure (Germano et al., 1991) by averaging over Lagrangian trajectories to determine the Smagorinsky coefficient. The upper boundary condition is stressfree, zero temperature gradient and no flow through the boundary and periodic boundary conditions are employed in the horizontal. A damping layer is also used near the top of the domain to prevent the reflection of gravity waves from the upper boundary. The wall model is based on imposing Monin–Obukhov similarity in a local sense.

A total of ten LES runs spanning a range of \(-h/L\) from 7.2–48.9 was conducted, where \( L = -u'_sw'\kappa g\overline{\theta} \) is the Obukhov length, \( \kappa \) is the von Kármán constant and \( u_s \) is the friction velocity. The LES domain was set to \( 12 \times 12 \times 2 \) km\(^3\) with a grid resolution of 160 × 160 × 160 (75 × 75 × 12.5 m\(^3\) in the x, y and z directions, respectively) and a time step of \( \Delta t = 0.05 \) s. The initial depth of the boundary layer was set to \( h = 1000 \) m, the simulations were forced by a constant pressure gradient expressed in terms of the geostrophic velocity \( U_g \) using the geostrophic approximation and a constant surface heat flux was imposed. The range of \(-h/L\) was obtained by systematically changing \( U_g \) between 9 and 15 m s\(^{-1}\) and \( \overline{w\theta} \) between 0.1 and 0.24 m s\(^{-1}\). Table 1 summarizes the properties of the ten simulations including the forcing, characteristic length (\(-L\) and \(h\)) and velocity (\(u_s\) and \(w_s\)) scales. These parameters are based on averages from hours 4–5 of the simulations. Examination of hourly averages of mean profiles showed that the moments are well converged after 4 h physical time, i.e. approximately 20 large eddy turnover times \((h/w_s)\). The height of the CABL \(h\) is defined as the location where the sensible heat flux is minimum \((\approx 0.2\overline{w\theta})\).

Figure 3 shows the LES-resolved profiles of the variances and third-order moments of \(w\) and \(\theta\) for the ten simulations, normalized by a combination of \((\overline{w_s}, \overline{\theta_s})\). Figure 4 is the same as Figure 3, but the profiles are normalized by \(\sigma_w, \sigma_\theta\) to show the moments \(M_k\). It is clear that the TOM are not simply related by constants, as noted by the wind tunnel experiment of Raupach (1981). While the moments \(M_{01}\) and \(M_{12}\) have fairly similar profiles, their gradients change sign at different heights in the mixed layer. This also applies for any one moment across the ten simulations, where the inflection point occurs at higher locations with increasing \(w_s/\overline{u_s}\). The skewness of vertical velocity, \(M_{03}\), is not constant in the mixed layer, as assumed by Wyngaard and Weil (1991), leading to their parametrization in Eq. (6). The terms in the heat-flux budget (Eq. (11)) are shown in Figure 5 for cases S1 and S10 for illustration. These cases are the end members of the LES simulations here, with S1 (\(w_s/\overline{u_s} = 4.93\)) and S10 (\(w_s/\overline{u_s} = 2.61\)) representing strongly and weakly convective simulations (see Table 1). These are obtained directly from the LES and the pressure term is calculated as a residual for the heat-flux budget. All the terms are comparable in the middle of the CABL (around \(z/h = 0.5\)) and the turbulent transport \(T\) becomes a source for heat flux comparable to the buoyancy term in this region.

4. Results and discussion

Using the overall statistics from the LES, a modified Rotta closure for the pressure gradient–potential temperature covariance term \((P)\) (Eq. (12)) and the singularity in the time-scale (and hence in \(\kappa_u\)) also noted by Wyngaard and Weil (1991) are first examined. The contribution of the local and non-local terms to the total heat flux in Eq. (13) is then presented, followed by an evaluation of the down-gradient diffusion closure to the flux-transport term with various turbulent diffusivity profiles. Finally, the asymmetry in the \((w, \theta)\) quadrant analysis quantified by the quantity \(\Delta F\) is investigated along with the relative roles of the TOM in contributing to this asymmetry. The EDCG,
TA, TOMP and EDMF model parametrizations are compared throughout.

4.1. The modified Rotta closure

Figure 6 shows a comparison between the LES output and the modelled pressure term ($P$). The latter uses the modified Rotta closure (MRC) in Eq. (12), with $h/\sigma_w$, $h/\sqrt{TKE}$ or $h/w_*$ as relaxation time-scales. The constants $C_1 = 3$, $C_2 = 1/2$ and $C_3 = 2/5$ are used. It is noticeable from Figure 6 that these time-scales do not result in significant differences in the modelled profile of $P$, due to the fact that the Rotta term in Eq. (12) is small relative to the buoyancy and mean gradient counterparts. Figure 6 also shows that, in both cases S1 and S10, the MRC reproduces the shape of the profile of $P$ obtained from the LES reasonably.

The return to isotropy time-scale $\tau_1$ obtained by rearranging Eq. (12) reads

$$\tau_1 = \frac{-C_1 \overline{w\theta}}{P + C_2 \beta \overline{\theta^2} - C_3 \sigma_w^2 (d\theta/dz)},$$

(25)

which shows that, for $C_2 = C_3 = 0$, i.e. for a simple Rotta closure for the term $P$, $\tau_1$ becomes negative in the regime $\overline{w\theta} < 0$. This remains the case even when including the buoyancy effects with $C_2 = 0.38$ (Deardorff, 1974) or $C_2 = 1/2$ (Moeng and Wyngaard,
The heat-flux budget terms in Eq. (11) normalized by the convective velocity and temperature scales and the boundary-layer height. The simulations with (a) the highest (S1) and (b) the lowest (S10) ratio of $w^*/u^*$ are shown for illustration. These simulations are described in Table 1.

The modified Rotta closure (MRC) model for the pressure gradient–temperature covariance term ($P$) from Eq. (12) with several profiles of the time-scale $\tau_1$ (see legend for the time-scales). The black line represents the term ($P$) obtained as a residual to the heat-flux budget (Eq. (11)) from the LES runs. Left and right columns are for simulations S1 and S10 respectively.

1986) and the mean-gradient term with $C_3 = 2/5$. The fact that the numerator and denominator in Eq. (25) change sign at different heights and in opposite directions leads to an apparent singularity in $\tau_1$ that was noted by Moeng and Wyngaard (1986) and Wyngaard and Weil (1991). This singularity was explained on the basis that bottom-up and top-down diffusion show different eddy-diffusivity profiles. However, these differences can be accommodated by adapting Eq. (25) to the negative flux portion of the CABL. Since the pressure term acts to decorrelate the vertical velocity and temperature, a change of sign of all terms is required in the negative heat-flux regime. This is equivalent to a downward-looking (top-down) perspective of the entrainment zone with a boundary condition $w_\theta \sim -0.2\Delta h_\theta$. Figure 7 shows the profiles of $\tau_1$ calculated from the LES and Eq. (25). Acceptable agreement with the corresponding profiles obtained by Moeng and Wyngaard (1986) for the heat flux is noted here, but Eq. (25) avoids separating the boundary layer into top-down and bottom-up mechanisms. Further, it is noticeable from Eq. (25) that $\tau_1 \sim 0$ when $\overline{w\theta} \sim 0$, unless the denominator is identically zero at the same height and then $\tau_1$ becomes indeterminate but still finite. The latter is the case in our LES runs, where the numerator and denominator approach zero at approximately the same height, i.e. with a difference less than $\Delta z/2$, where $\Delta z = 12.5 \text{ m}$ is the vertical resolution. Such a difference can be attributed to numerical artifacts; in particular, the term $P$ is obtained here as a residual to the heat-flux budget and thus incorporates all the uncertainties.

4.2. Local closure approach for the flux-transport term

As mentioned earlier, the model in Eq. (13) can be used to evaluate the local (first term) and non-local (last two terms) contributions.
to the total heat flux. First, the performance of this model in reproducing the heat flux obtained from the LES is shown in the top panel of Figure 8. The vertical profile of the modelled flux (black line) is obtained using Eq. (13) with a relaxation time-scale $\tau_1 = h/\sigma_w$, but other time-scales such as $h/\sqrt{TKE}$ or $h/\sigma_w$ show comparable performance, as noted in section 4.1. Since all the terms in Eq. (13) are obtained from the LES, except $\tau_1$ and the constants, the deviations between modelled and LES fluxes are due mostly to the performance of the MRC (relaxation time-scale $\tau_1$).

While this remains beyond the scope of this article, it is important to consider height-dependent rather than constant values of $C_2$ and $C_3$ in Eq. (12) (see a recent article by Heinze et al., 2016). The bottom panel of Figure 8 shows the contribution of each term in Eq. (13) to the total heat flux. The gradient diffusion term ($\propto d\Theta/dz$) becomes negative in the middle of the CABL, emphasizing the counter-gradient transport. It is noticeable that the sum of the non-local contributions to the heat flux, $\overline{w\theta}_{NL}$, exceeds their local counterpart in almost all of the CABL and that the buoyancy and flux-transport terms are comparable to each other.

The solution of Eq. (16) is shown in Figure 9 for simulations S1 and S10. Several profiles of the eddy diffusivity $K_T = \tau_2 q^2$ are tested. With $q^2 \propto \sigma_w^2$, the profiles of $\tau_2$ are $L_B/\sigma_w$, $L_B/\sqrt{TKE}$, $h/\sigma_w$ and $h/\sqrt{TKE}$, where $L_B$ is the Blackadar length-scale, defined by (Blackadar, 1962)

$$L_B = \frac{kz}{1 + kz/L_0},$$

where $k \sim 0.4$ is the von Kármán constant and $L_0$ is an asymptotic value given by

$$L_0 = \frac{\alpha_b}{\int_0^h qz \, dz},$$

with $\alpha_b = 0.1$ (Mellor and Yamada, 1974) and $q = \sigma_w$ here. Figure 9 shows that the CABL height $h$ performs relatively better than $L_B$ as a length-scale for the profile of $K_T$, particularly in the strongly convective case S1. An eddy diffusivity with the Blackadar length-scale underestimates the heat flux in the bottom of the CABL, but performs comparably to that with $h$ as a length-scale in the upper half as $L_B$ approaches $L_0$. The time-scale $\tau_2 = h/\sigma_w$, which is equivalent to the Lagrangian time-scale $T_L$ used by Wyngaard and Weil (1991), performs best with $q^2 = \sigma_w^2$. Using $q^2 = TKE$ did not result in significant differences (not shown).

4.3. Transport asymmetry and the ejection-sweep events

The results of the quadrant analysis of the ($w, \theta$) events are shown in Figure 10 for the end-member cases S1 and S10. This conditional sampling technique represents the average number of events of ($w, \theta$) jointly occurring in quadrant $i$. The averaging time here is 4 h and the sampling is conducted at each height (layer) of the CABL. Note that the quantity $F_i$ in Eq. (20) has a singularity when $\overline{w\theta} \sim 0$ and hence the top panel of

![Figure 7. Return to isotropy time-scale, normalized by the large-eddy turnover time-scale ($h/w_*$) and calculated from the LES profiles (Eq. (25)) for simulations S1, S5 and S10.](image)

![Figure 8. (a, b) Comparison of the heat-flux profiles obtained from the LES output (blue dots) and from the model in Eq. (13) with $\tau_1 = h/\sigma_w$ (black dots). (c, d) Contribution of each term (normalized by $w_*\theta_*$) in Eq. (13) to the modelled heat flux. Left and right columns are for simulations S1 and S10, respectively.](image)
Figure 9. Comparison of the modelled heat flux profiles (normalized by surface heat flux) using Eq. (16) with the LES output (black line). The modelled profiles (red, blue, green and magenta dots) are obtained using different eddy-diffusivity ($K_T$) profiles in Eq. (16) (see legend). $L_B$ is the Blackadar length-scale (see text). (a) and (b) are for simulations S1 and S10, respectively.

Figure 10. Conditional sampling and quadrant analysis of the ($w$, $\theta$) scatter plot from the LES output. (a, b) The fractional contributions $\langle w\theta \rangle_i$ of each quadrant ($i = I, II, III$ and IV) to the total heat flux (see Figure 2 for definition of quadrants). (c, d) The imbalance in these contributions quantified by $\Delta F_0 = R\Delta F$ (see text in section 4.3). Left and right columns are for simulations S1 and S10, respectively.

Figure 10 shows the contribution $\langle w\theta \rangle_i = F_i \overline{w\theta}$ of each quadrant to the total heat flux. Quadrant I is associated with rising warm air (ejections) due to positive buoyancy and clearly has the largest contribution to the positive heat flux. Nevertheless, the contribution of subsiding cold air parcels in quadrant III (sweeps) to this positive flux is not negligible. Near the top of the boundary layer, quadrants II (entrained warm air) and IV (rising cold air) have more pronounced contributions to the heat flux. An important perspective that this analysis emphasizes is the fact that the updraughts in EDMF models and/or bottom-up diffusion in TA models can carry negative temperature fluctuations upward (quadrant IV) and that downdraughts (top-down) can transport positive temperature fluctuations downward (quadrant II). It is also noticeable that in the lower part of the CABL, where $\overline{w\theta} > 0$, quadrants II and IV still contribute to the heat flux and hence account for the effects of top-down diffusion over the entire depth of the boundary layer. The same applies for quadrants I and III in the negative heat-flux portion (upper 20% of the CABL), which indicates that the updraughts/downdraughts and bottom-up/top-down mechanisms are not decoupled in their contribution to the net heat flux. Quadrant analysis can then be perceived as a more general framework for examining these individual mechanisms. The bottom panel of Figure 10 shows the imbalance between the contributions of ejections and sweeps to the heat flux, i.e. quadrants I and III when $\overline{w\theta} > 0$ and quadrants II and IV when $\overline{w\theta} < 0$. Note that the quantity $\Delta F$ in Eq. (22)
does not have a singularity when $\theta' \sim 0$, since sweeps and ejections balance at the same height and hence the numerator becomes zero. For illustration purposes, the quantity plotted in Figure 10 is $\Delta F_0 = RA F_0$, where $R$ is the correlation coefficient. This quantity is negative in most of the CABL, indicating that ejections are dominant over sweeping events for the positive heat-flux regime. When $\Delta F_0$ becomes positive near the top, $R$ switches sign and quadrant II contributes more to the downward heat flux than quadrant IV. This asymmetry in heat transport between the different quadrants becomes stronger with increasing $w_{\ast}/u_{\ast}$, where case S1 shows the highest absolute value of $\Delta F_0$.

Connections between the asymmetry and the TOM can be achieved through Eq. (23). This truncation at third-order of $J(w, \theta)$ appears sufficient to capture the asymmetry quantified by quadrant analysis (Figure 11). While the expansion in Eq. (23) slightly underestimates the magnitude of $\Delta F_0$ (Figure 11), it reproduces the overall profile reasonably and, although this asymmetry increases with stronger convection (red lines in Figure 11), $\Delta F_0$ seems to attain a ‘self-similar’ shape with increasing $w_{\ast}/u_{\ast}$. Note that $\Delta F$ and $\Delta F_0$ are bounded between $-1$ (pure ejection flow) and $+1$ (pure sweeping flow). Nevertheless, despite being comprehensive, Eq. (23) remains taxing, since it involves the correlation coefficient $R$ and the four TOM ($M_3$) that require parametrization. Katul et al. (1997) and later Cava et al. (2006) noted that the first term in this cumulant expansion [$\propto (M_{03} - M_{30})$] may be small compared with the contribution of the mixed moments. The same analysis is repeated here in Figure 12, which indicates that the ejection-sweep events and transport asymmetry are attributed to the fact that turbulence transports heat flux and air-temperature variance differently. The right panel of Figure 12 shows a comparison of the quantity $\Delta F_0$ calculated from the full expansion in Eq. (23) and from the mixed momen term $[(1/2)\sqrt{2\pi}](M_{21} - M_{12})$ only. Furthermore, it is interesting to note that this latter result would appear in its exact form if the TOM parametrization in Eqs (7) and (8) by Abdella and McFarlane (1997) with the correction by Mironov et al. (1999), namely $M_{03} = S_{w} = \bar{w} \theta'/\langle \sigma_{w} \sigma_{\theta'} \rangle$ and $M_{30} = S_{\theta} = \bar{w} \theta' / \langle \sigma_{w} \sigma_{\theta'} \rangle$, were substituted in Eq. (23). After some rearrangement and ignoring the contribution of the difference in skewness term ($\propto M_{03} - M_{30}$), Eq. (23) can be written as

$$\bar{w} \theta' = \sigma_{w} \sigma_{\theta'} / \pi \sigma_{\theta} = 2 \sqrt{\pi} \sigma_{w} \Delta F \bar{w} \theta'$$

and, using Eq. (8), the flux-transport term then reads

$$\frac{d \bar{w} \theta'}{dz} = \frac{d}{dz}(S_{(w, \theta)} \sigma_{w} \bar{w} \theta') = 2 \sqrt{\pi} \left( \sigma_{w} \Delta F \bar{w} \theta' \right),$$

where $S_{(w, \theta)}$ can be $S_{w}$ as originally suggested by Abdella and McFarlane (1997) in Eq. (8) or $S_{\theta}$ after Mironov et al. (1999). Recall that the first term on the rhs of Eq. (29), if $S_{w}$ is used for $S_{w, \theta}$, is equal to $d \bar{w} \theta'/dz$ from Eq. (7) and hence the model by Abdella and McFarlane (1997) is equivalent to an approximation for the JPDF such that $\Delta F = 0$ when $\theta' \neq 0$. An equally important note is a comparison with the model of non-local flux ($\bar{w} \theta'_{NL}$) by Wyngaard and Weil (1991) in Eq. (6). This model can be recovered from Eq. (29) by setting $\Delta F = 0$ and $S_{w}$ and $\sigma_{w}$ as constants, which was assumed by Wyngaard and Weil (1991). The flux-transport term appears in the flux budget as $(C_{3} - 1)\tau_{1} / C_{3} \bar{w} \theta'/dz$, and hence $\tau_{1} = T_{L} = h / \sigma_{w}$ here. Next, we consider the following relation between the two mixed TOM, $\bar{w} \theta' = C(z) \bar{w} \theta'$, where $C(z)$ is not constant. For instance, $C(z) = \sigma_{w} / \sigma_{w}$ in the parametrization of Abdella and McFarlane (1997), which would lead to $\Delta F = 0$ in Eq. (28),

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure11.png}
\caption{Comparison of the quantity $\Delta F_0$ from (a) conditional sampling (quadrant analysis) and (b) the cumulant expansion in Eq. (23). Red colours are for simulations S1–S4, blue for S5–S7 and black for S8–S10. (c) The quantity $\Delta F_0$ calculated from cumulant expansion in Eq. (23) ($y$-axis) and quadrant analysis ($x$-axis). The 1:1 line (black) in the bottom figure (c) is shown for reference.}
\end{figure}
and $C(z) = S_0 \sigma_\theta / S_w \sigma_w$ with the correction of Mironov et al. (1999). Introducing $B(z) = 1 - C(z) \sigma_\theta / \sigma_w$, Eq. (28) can now be written as

$$\frac{\overline{w \theta'}}{\overline{\theta'}} = - \frac{2 \sqrt{2\pi}}{B(z)} \sigma_\theta \Delta F \overline{w \theta'},$$

which defines an alternative parametrization for the turbulent flux of heat that explicitly encodes the role of ejections and sweeps in the corresponding budget. While Eq. (30) serves no prognostic purpose, since the profile of $\Delta F$ is not known a priori (but is not zero), it remains useful in diagnosing the failure of the conventional gradient-diffusion model and in incorporating the role of large-scale motion in contributing to the sensible heat flux. If the representation of $\overline{w \theta'}$ in Eq. (30) and its downgradient-diffusion counterpart in Eq. (15) are compared, the quantity $\Delta F$ can be expressed as

$$\Delta F = \frac{h (d \overline{w \theta'}/dz) B(z)}{2 (\sqrt{2\pi}/\overline{w \theta'}),}$$

where $\tau_2 = h/\sigma_w$ and $\hat{q}^2 = \sigma_w^2$ are used, as noted earlier. By analogy with Eq. (22) and since $h$ and $d \overline{w \theta'}/dz$ are constant, Eq. (31) shows that the imbalance $\langle \overline{w \theta'} \rangle_{sweeps} - \langle w \theta' \rangle_{ejections}$ scales with $B(z)$, i.e. the asymmetry in temperature variance and flux transport mechanisms. While this conclusion has been alluded to earlier by ignoring the skewness term and retaining the term $\propto (M_1 - M_2)$ (see Eq. (28)), the latter comparison in Eq. (31) represents an independent confirmation of this result. With the parametrization in Eq. (30), the heat-flux budget in Eq. (13) can be written as a first-order differential equation of the form

$$A_1(z) \frac{d \overline{w \theta'}}{dz} + A_2(z) \overline{w \theta'} = A_3(z),$$

which has the general solution

$$\overline{w \theta'} = \frac{A_3}{A_1} \left[ 1 - \exp \left( - \frac{A_2}{A_1} z \right) \right] + C_1,$$

where $C_1$ is an integration constant set by the boundary condition $\overline{w \theta'}_{z=0} = \overline{w \theta'}_0$. To explore the characteristics of this solution, consider the case where $A_2/A_1$ and $A_3/A_1$ are non-zero constants. This is equivalent to assuming that the quantity $\overline{w \theta'}/\overline{\theta'} \sim \sigma_w \Delta F/B(z)$ and its gradient that appears in $A_2$ scale with the mean gradient ($M$) and the buoyancy ($B$) terms in $A_3$, which can be seen in the flux budget Eq. (11) with the MRC for the pressure term. The general solution in Eq. (33) then becomes

$$\overline{w \theta'} = \frac{A_3}{A_1} z - \frac{A_2 A_3}{A_1^2} \frac{z^2}{2} + \ldots + \overline{w \theta'}_0$$

and hence for a linear flux profile, i.e. truncating the expansion at first order, the ratio $A_3/A_1 < 0$ sets a slope of $\overline{w \theta'}$. Recall that we initially assumed that $A_3/A_1$ is a non-zero constant. Since $(\overline{w \theta'})_{z=h} = \overline{w \theta'}_0$, it also follows that

$$\frac{A_3}{A_1} = \frac{\overline{w \theta'}_0 - \overline{w \theta'}}{h},$$

which shows that the entrainment flux is related to the asymmetry between ejections and sweeps. Explicit connections between EDMF models and the JPDF are considered next.
4.4. Analogy between EDMF models and the relaxed eddy accumulation method

The convective mass-flux term in EDMF models, equivalent to \( w \theta (\|) \) in EDMF (Equation (10)), with \( M = a_1(\| - \bar{\|}) \) appears to bear some similarity to the relaxed eddy accumulation (REA) method used in scalar flux measurements near the surface (e.g. Businger and Oncley, 1990; Katul, 1994). The REA relies on conditional sampling of updraughts (rising air parcels) and downdraughts (subsiding parcels) to estimate a scalar flux as

\[
\bar{w} \theta = b \sigma_w \left( \Theta_\theta - \Theta_- \right),
\]

(37)

where the potential temperature fluctuations are used as the scalar of interest here, \( b \approx 0.52–0.62 \) (Kut et al. 1996) is a proportionality constant and \( \Theta_\theta \) (equivalent to \( \Theta_\theta \)) and \( \Theta_- \) (equivalent to \( \Theta_- \)) are the mean temperatures in the updraughts and downdraughts, respectively. Recall that \( \Theta = \Theta_\theta \) and \( \| = \|_w \) in the EDMF models are only approximations of the fact that the updraughts occupy a narrow area and are surrounded by a slowly subsiding environment; hence, by analogy, mass flux \( M \sim b \sigma_w \). This was also noted by Wyngaard and Moeng (1992) and, in another context, Siebesma et al. (2007) used the approximation \( b \approx 0.3 \). Starting with a Gaussian JPDF of \( \|/\theta_\theta \) and \( \|/\sigma_w \), with the normalized temperature and vertical velocity plotted on the y- and x-axes respectively (see Figure 2), then the correlation coefficient can be approximated by

\[
R = \frac{(\Theta_\theta - \Theta_-) / \sigma_\theta}{(\| - \bar{\|}) / \sigma_w},
\]

(38)

where \( \| = \|_w = \bar{\|} \) are the mean vertical velocity components in the updraughts and downdraughts, respectively. Using \( \bar{w} \theta = R \sigma_w \sigma_\theta \), the heat flux is given by

\[
\bar{w} \theta = \frac{\sigma_w}{\| - \bar{\|}} \frac{\sigma_\theta}{\Theta_\theta - \Theta_-},
\]

(39)

and, by analogy to Equation (37), the coefficient \( b \) is given as

\[
b = \frac{\sigma_w}{\| - \bar{\|}},
\]

(40)

These relations, originally developed by Baker et al. (1992), are used in many contexts. With this assumption, the mass flux is

\[
M = a_1 (\| - \bar{\|}) = \frac{\sigma_w}{\| - \bar{\|}} \sigma_w
\]

and hence the fractional area occupied by the updraughts as \( a_1 \sim b^2 \). This area is 0.09 for the value \( b = 0.3 \) used by Siebesma et al. (2007) and ranges between 0.27 and 0.38 for the usual values of \( b \approx 0.52–0.62 \). Hence, it can be surmised that the EDMF models are based on a quasi-Gaussian approximation to the JPDF for the normalized \( \|/\sigma_w \) and \( \|/\sigma_\theta \) or, equivalently, setting \( \Delta F_\| = 0 \).

5. Conclusions

Various models that correct down-gradient diffusion approximations in the convective atmospheric boundary layer (CABL) employ a counter-gradient (EDCG), transport asymmetry (TA), third-order moment parametrization (TOMP) or mass-flux (EDMF) approach. Reconciling such models and unfolding their similarities has resisted complete theoretical treatment. Using LES runs for the CABL, the role of the turbulent flux-transport term and its contribution to the sensible heat-flux budget was examined, which revealed that the third-order moments do shape such non-local effects. First, a modified Rotta closure for the pressure gradient–potential temperature term and a down-gradient diffusion approach for closing the flux-transport term were evaluated with a variety of closure time- and length-scales. The analysis indicates that the height of the CABL and the vertical velocity variance are acceptable closure length and velocity scales. Second, a diagnostic framework that reveals the role of the third-order moments in shaping the asymmetry in vertical diffusion of scalars in the CABL was developed and characterized. This framework relies on conditional sampling and quadrant analysis of the JPDF of vertical velocity and potential temperature, which is indicative of the contributions of each quadrant and physical flow mechanism to the total heat flux. The imbalance between these quadrants is tied to ejections and sweeps in the flow field and was expanded in terms of the third-order moments of the Gram–Charlier expansion of the JPDF. The EDCG, TA, TOMP and EDMF models were linked to different approximations of the JPDF, particularly to assumptions regarding the asymmetry and imbalance between ejections and sweeps. This imbalance is due mostly to the mixed moments rather than the skewness. For instance, the EDCG model that parametrizes the third moments in terms of bulk properties of the CABL can be viewed as an integrated approach of such asymmetry. Both TA and TOMP models were retrieved by neglecting the quantity \( \Delta F_\| \), the imbalance between ejections and sweeps, and assuming height-independent vertical profiles of the skewness and variance of vertical velocity. The EDMF model was shown to follow from a Gaussian approximation to the JPDF, in line with REA methods. An interesting connection between the coefficient \( b \) in REA and the fractional area \( a_1 \) occupied by the updraughts suggested that the latter is not necessarily negligible, as assumed by EDMF models. This may indicate that the negated term \( a_1w \theta \) may still be important and, together with the term \( (1 - a_1)w \theta \), may be responsible for local fluxes in updraughts and the surrounding environment, respectively, with eddy diffusivities weighted by the fractional area \( a_1 \). Finally, the LES runs suggest that the \( \Delta F_\| \) profiles appear to reach a self-similar shape (depending only on \( z/h \), offering the possibility of a novel closure model for the heat-flux budget in the CABL.

Acknowledgements

K. Ghannam and G. Katul acknowledge support from the National Science Foundation (NSF-CBET-103347 and NSF-EAR-1344703), the US Department of Energy (DOE) through the office of Biological and Environmental Research (BER) Terrestrial Ecosystem Science (TES) Program (DE-SC0006967 and DE-SC0011461) and the Duke University WISENet Program sponsored by the National Science Foundation (Grant DEG-1068871).

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