Connecting the Failure of K Theory inside and above Vegetation Canopies and Ejection–Sweep Cycles by a Large-Eddy Simulation

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ABSTRACT

Parameterizations of biosphere–atmosphere interaction processes in climate models and other hydrological applications require characterization of turbulent transport of momentum and scalars between vegetation canopies and the atmosphere, which is often modeled using a turbulent analogy to molecular diffusion processes. Simple flux–gradient approaches (K theory) fail for canopy turbulence, however. One cause is turbulent transport by large coherent eddies at the canopy scale, which can be linked to sweep–ejection events and bear signatures of nonlocal organized eddy motions. The K theory, which parameterizes the turbulent flux or stress proportional to the local concentration or velocity gradient, fails to account for these nonlocal organized motions. The connection to sweep–ejection cycles and the local turbulent flux can be traced back to the turbulence triple moment $\overline{c'w'w'}$. In this work, large-eddy simulation is used to investigate the diagnostic connection between the failure of K theory and sweep–ejection motions. Analyzed schemes are quadrant analysis and complete and incomplete cumulant expansion methods. The latter approaches introduce a turbulence time scale in the modeling. Furthermore, it is found that the momentum flux and sensible heat flux need different formulations for the turbulence time scale. Accounting for buoyancy in stratified conditions is also deemed important in addition to accounting for nonlocal events to predict the correct momentum or scalar fluxes.

1. Introduction

It is a standard practice in modeling land surface–atmosphere interaction that momentum or scalar fluxes can be parameterized by relating them to the mean velocity gradient or scalar concentration gradient by means of a turbulent diffusion coefficient, called gradient–diffusion parameterization or K theory (Raupach and Thom 1981; Katul et al. 2013). The K theory has enjoyed a high degree of popularity over the years, especially because of the ease of usage. It has been found to be inadequate in vegetation canopies, however, which was demonstrated by Denmead and Bradley (1985) by means of detailed scalar flux and concentration measurements. Denmead and Bradley (1985), as summarized in Cava et al. (2006, p. 218), reported that a cogradient flow of

heat, water vapor, and carbon dioxide exists near the canopy top but in the middle and lower levels of the canopy zero or countergradient flow can exist (see also Shuttleworth and Gurney 1990). Several reasons can be identified for the failure of simple K theory inside canopies [see Cava et al. (2006, p. 218) for a summary and other references], among which there are three main ones (Wilson and Shaw 1977; Raupach 1989; Finnigan 2000). Katul et al. (2013, section 6.2) list them as follows: 1) “variable scalar source distribution within the canopy strongly impacts the apparent diffusivity (near-field effects),” 2) “lack of local balance between turbulent production and dissipation (unlike the atmospheric surface layer),” and 3) “vertical transport occurs by (organized) eddy motion whose size is comparable to [the canopy height], which is larger than the scale at which the mean concentration gradients change.” Alternatives for K theory take care of the near-field effects of scalar sources by the Lagrangian localized near-field theory (LNF) as described by Raupach (1989) and Siqueira et al. (2000) and higher-order Eulerian closure models (Wilson and Shaw 1977). Katul and Albertson (1999) resolved the

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imbalance between production and dissipation by assuming a gradient-diffusion parameterization for higher-order mixed moments. However, “the role of large-scale coherent motion remained implicit to these two approaches” (Katul et al. 2013, section 6.2). Then, over the past two decades, a multitude of work has been published in which attempts were made to link the large-scale organized eddy motions to countergradient (or zero gradient) flows within plant canopies (Wilson and Shaw 1977; Finnigan 1979; Raupach and Thom 1981; Raupach 1989; Gao et al. 1989; Shaw et al. 1989; Wilson 1989; Leclerc et al. 1990, 1991; Kaimal and Finnigan 1994; Finnigan 2000; Cava et al. 2006). Furthermore, since the publication of several studies (Shaw and Schumann 1992; Kanda and Hino 1994; Dwyer et al. 1997; Su et al. 1998; Fitzmaurice et al. 2004; Ross 2008; Dupont and Brunet 2009; Patton and Katul 2009), large-eddy simulation (LES) has become a standard tool for investigating canopy turbulence.

In this work, we use an LES to study the linkage between the nonlocal effects and failure of K theory inside vegetation canopies. Our focus extends up to the canopy sublayer (i.e., up to 2–6 times the canopy height). We first revisit the standard theory in the literature (section 2), recapitulating the budgets for momentum and sensible heat flux, commenting on the choice of turbulence time scale, and expounding on the quadrant analysis of sweep–ejection events. We then describe our simulation setup (section 3) and verify the correct behavior of our simulated data. Next, we evaluate K theory in and above the canopy, compare it with more elaborate approaches, and connect its failure with the sweep–ejection cycles (section 4).

2. Theory

For a stationary, planar–homogeneous flow without subsidence and with high Peclet and Reynolds numbers, the spatiotemporally averaged momentum and scalar (e.g., heat) flux budget equations are written as (Raupach et al. 1986; Zhuang and Amiro 1994; Cava et al. 2006; Katul et al. 2013)

$$\frac{\partial \overline{w'u'}}{\partial t} = 0 = -\overline{w'w'} \frac{\partial \overline{U}}{\partial z} - \frac{\partial (\overline{w'w'u'})}{\partial z} + \frac{g}{T} \overline{u'T'} - \frac{1}{\rho} \left(u' \frac{\partial p'}{\partial z} \right) \quad \text{and} \quad (1)$$

$$\frac{\partial \overline{w'T'}}{\partial t} = 0 = -\overline{w'w'} \frac{\partial \overline{T}}{\partial z} - \frac{\partial (\overline{w'w'T'})}{\partial z} + \frac{g}{T} \overline{T'T'} - \frac{1}{\rho} \left(T' \frac{\partial p'}{\partial z} \right), \quad (2)$$

where u and w denote the horizontal and vertical velocities, an overbar denotes the space and time double-averaging operator; $\overline{U}$ denotes the mean streamwise velocity, $\overline{T}$ denotes mean potential temperature, and w' , u' , and T' denote vertical and horizontal turbulent velocity fluctuations and the potential temperature fluctuations from their corresponding double-averaged means. In addition, $\overline{w'u'}$ and $\overline{w'T'}$ denote the turbulent momentum flux and sensible heat flux, respectively. The horizontal coordinate x is aligned with the mean wind; z is the vertical coordinate, p' is the turbulent pressure fluctuation, g is gravitational acceleration, and ρ is mean air density. The terms on the right-hand side (rhs) of Eqs. (1) and (2) are the flux production, turbulent transport, pressure–velocity (and pressure–scalar) interaction, and buoyant production, respectively. It is important to note here that the effects of viscous dissipation and canopy drag effects on the momentum and scalar flux budgets are small and can be safely neglected (Raupach et al. 1986; Zhuang and Amiro 1994). The pressure–velocity interaction term in Eq. (1) is a decorrelation term, and it can be parameterized using principles of second-order closure modeling as

$$\frac{1}{\rho} \left(u' \frac{\partial p'}{\partial z} \right) = \frac{C_R}{\tau} (\overline{w'u'}) - C_1 (\overline{w'w'}) \frac{\partial \overline{U}}{\partial z}, \quad (3)$$

where $\tau = \kappa/\varepsilon$ is a relaxation time scale to be discussed in detail in section 2a, κ is the turbulent kinetic energy (TKE), ε is the dissipation rate of κ , $C_R \approx 1.8$ is known as the Rotta constant, and $C_1 = 3/5$ is a constant that is associated with the isotropization of the production term correcting the original Rotta model (see the appendix for more details) and is consistent with rapid distortion theory (Choi and Lumley 2001; Pope 2000; Banerjee et al. 2013; Katul et al. 2013). This model/term along with its associated two constants is referred to as the Launder–Reece–Rodi approach with isotropization of the production (Launder et al. 1975). By using Eq. (3), Eq. (1) can be written as

$$\overline{w'u'} = \frac{\tau}{C_R} \left[(C_1 - 1) \overline{w'w'} \frac{\partial \overline{U}}{\partial z} - \frac{\partial (\overline{w'w'u'})}{\partial z} + \frac{g}{T} \overline{u'T'} \right]. \quad (4)$$

In a similar way, the pressure–scalar interaction term in Eq. (2) can be modeled as

$$\frac{1}{\rho} \left(T' \frac{\partial p'}{\partial z} \right) = \frac{C_2}{\tau} (\overline{w'T'}) - \beta \frac{g}{T} (\overline{T'T'}), \quad (5)$$

where $C_2 \approx 2.5$ – 3.0 is a closure constant and the τ here is an Eulerian relaxation time scale, also discussed in section 2a. There is some debate about the value of the parameter β , which is reported to range from $-1/2$ to $1/3$

(Wyngaard 1984; Ghannam et al. 2016; Katul et al. 2016). By using Eq. (5), Eq. (2) can be written as

$$\frac{\overline{w'T'}}{C_2} = \frac{\tau}{C_2} \left[-\overline{w'w'} \frac{\partial \overline{T}}{\partial z} - \frac{\partial (\overline{w'w'T'})}{\partial z} + (1 + \beta) \frac{g}{T} \overline{T'T'} \right]. \quad (6)$$

It is important to note here that in the absence of the triple moment (second term on the rhs) and the buoyancy term (third term on the rhs), Eqs. (4) and (6) are left with the gradient-diffusion parameterization (or K theory) where the flux $F = K \partial \overline{U} / \partial z$ or $F = K \partial \overline{T} / \partial z$, that is, a diffusivity multiplied by the gradient of velocity or temperature. In these cases, the diffusivity attains a general form of $K = (\tau/C) (\overline{w'w'})$, where C is an arbitrary constant. Hence, from Eqs. (4) and (6) it can be stated that the failure of K theory is associated with neglecting the triple-moment and buoyancy terms. Moreover, as will be discussed in section 2b, because the triple moment can be linked with large-scale nonlocal organized motions, a connection between the failure of K theory and sweep–ejection cycles can be established. Evaluating that connection, however, requires a prescription for the relaxation time scale τ , which is discussed in section 2a.

a. Discussion on the relaxation time scale

Closure modeling of canopy sublayer turbulence requires specification of empirical characteristic principal time (or length) scales (Katul and Albertson 1999). The model by Wilson (1988) suggested the relaxation time scale $\tau = \kappa/\varepsilon$ that is based on the ratio between the TKE κ and the mean dissipation rate ε ; τ can be interpreted as a measure of how fast the turbulence comes into equilibrium with the local mean gradients (Belcher and Hunt 1998) or how quickly the energetic eddies degenerate and lose their coherence (Katul et al. 2013). Because the nonlocal coherent structures contribute to the TKE, they should have some representation in τ . Note that both the TKE and ε can be obtained from the LES output.

Another estimate that is based on a mixing-length argument was suggested by Poggi et al. (2006) and is given by

$$\tau = \begin{cases} \beta \frac{h_c}{\sigma_w} & \text{for } z/h_c \leq 0.75 \\ \frac{\kappa(z-d)u_*}{\sigma_w^2} & \text{for } z/h_c \geq 0.75 \end{cases}, \quad (7)$$

where now $\kappa = 0.4$ is the von Kármán constant, β is a parameter estimated to be about 0.1 for dense canopies, h_c is the canopy height, and d is the zero-plane displacement height, which can be taken as $(2/3)h_c$. Moreover, τ can also

be estimated directly using the Rotta Eqs. (3) and (5). This would suggest that three different estimates of τ are possible for momentum and heat, assuming that the same relaxation time scale governs both quantities. These different estimates will be discussed later in section 4.

b. Connection between the triple moment and sweep–ejection cycles

The sweep–ejection cycles associated with quadrant analysis have been extensively discussed in the turbulence literature (Antonia 1981; Katul et al. 2006; Wallace 2016) and are only briefly repeated here for the sake of completion. For a negative momentum or scalar flux ($\overline{w'c'} < 0$), where c' is u' or T' , sweeps and ejections are defined on the basis of a quadrant system where the abscissa is the scalar or horizontal velocity fluctuation c' and the ordinate is the vertical velocity fluctuation w' . Fluxes residing on quadrant II ($c' < 0$ and $w' > 0$) are called ejections and fluxes falling into quadrant IV ($c' > 0$ and $w' < 0$) are called sweeps. Events in the other two quadrants (quadrant I with $c' > 0$ and $w' > 0$ and quadrant III with $c' < 0$ and $w' < 0$) are called outward and inward interactions, respectively. Sweeps and ejections are found to be the major mechanisms of momentum or scalar flux transfer in the boundary layer. The difference between the sweeps and ejection components of the fluxes is a quantity of interest and is defined as (Nakagawa and Nezu 1977; Antonia 1981)

$$\Delta S_0 = \frac{\overline{w'c'_{IV}} - \overline{w'c'_{II}}}{\overline{w'c'}}, \quad (8)$$

where $\overline{w'c'_{IV}}$ and $\overline{w'c'_{II}}$ are the sweep and ejection components of the fluxes, respectively; $\Delta S_0 \geq 0$ indicates momentum transfer is sweep dominated, and $\Delta S_0 \leq 0$ would mean that momentum transfer is ejection dominated. Using the Gram–Charlier cumulant expansion method (CEM) truncated to third order as demonstrated by Frenkiel and Klebanoff (1967) and Raupach (1981), ΔS_0 can be expanded in terms of triple moments as (Katul et al. 2013)

$$\Delta S_0 = \frac{1 + R_{wc}}{R_{wc} \sqrt{2\pi}} \left[\frac{2C_A}{(1 + R_{wc})^2} + \frac{C_B}{(1 + R_{wc})} \right], \quad (9)$$

where

$$C_A = (1 + R_{wc}) \left[\frac{1}{6} (M_{03} - M_{30}) + \frac{1}{2} (M_{21} - M_{12}) \right] \quad (10)$$

and

$$C_B = - \left[\frac{1}{6} (2 - R_{wc}) (M_{03} - M_{30}) + \frac{1}{2} (M_{21} - M_{12}) \right]. \quad (11)$$

Here, $R_{wc} = \overline{w'c'}/(\sigma_w\sigma_c)$ and $M_{ij} = \overline{c'^i w'^j}/(\sigma_c^i \sigma_w^j)$. Thus, when $c = T$,

$$\begin{aligned} M_{03} &= \frac{\overline{w'w'w'}}{\sigma_w^3}; & M_{30} &= \frac{\overline{T'T'T'}}{\sigma_T^3}; \\ M_{21} &= \frac{\overline{T'T'w'}}{\sigma_T^2 \sigma_w}; & M_{12} &= \frac{\overline{T'w'w'}}{\sigma_T \sigma_w^2}. \end{aligned} \quad (12)$$

Moreover, it has been demonstrated by [Poggi et al. \(2004a\)](#), [Cava et al. \(2006\)](#), and [Katul et al. \(2013\)](#) that the skewness terms M_{03} and M_{30} do not contribute significantly toward ΔS_0 and that, under this “incomplete third-order cumulant expansion method” (ICEM) in which only the mixed triple moments contribute toward ΔS_0 ,

$$\Delta S_0 \approx \frac{1}{2R_{wc}\sqrt{2\pi}}(M_{21} - M_{12}). \quad (13)$$

Furthermore, as suggested by [Cava et al. \(2006\)](#) on the basis of experimental evidence, M_{12} and M_{21} are often related linearly for dense canopies, say by a proportionality constant $\gamma + 1$, thus expressing ΔS_0 only in terms of one mixed moment, which gives the following expression for the mixed moment:

$$M_{12} = \frac{\overline{c'w'w'}}{\sigma_c \sigma_w^2} \approx \frac{2\sqrt{2\pi}R_{wc}}{\gamma} \Delta S_0. \quad (14)$$

Combining Eq. (14) with the momentum budget [Eq. (4)] and heat budget [Eq. (6)] expressions yields

$$\begin{aligned} \overline{w'u'} &= \frac{\tau}{C_R} \left[(C_1 - 1) \overline{w'w'} \frac{\partial \bar{U}}{\partial z} \right. \\ &\quad \left. - \frac{\partial}{\partial z} \left(\frac{2\sqrt{2\pi}\sigma_u \sigma_w^2 R_{wu}}{\gamma} \Delta S_0 \right) + \frac{g}{T} \overline{u'T'} \right] \end{aligned} \quad (15)$$

and

$$\begin{aligned} \overline{w'T'} &= \frac{\tau}{C_2} \left[-\overline{w'w'} \frac{\partial \bar{T}}{\partial z} - \frac{\partial}{\partial z} \left(\frac{2\sqrt{2\pi}\sigma_T \sigma_w^2 R_{wT}}{\gamma} \Delta S_0 \right) \right. \\ &\quad \left. + (1 + \beta) \frac{g}{T} \overline{T'T'} \right]. \end{aligned} \quad (16)$$

Equations (15) and (16) are significant because they can relate the perturbation to the gradient-diffusion parameterization, to nonlocal transport events like sweeps and ejections ([Poggi and Katul 2007](#)), and also to the non-Gaussian nature of the joint probability distribution function between w' and c' , which is a characteristic feature of canopy turbulence. It is

important to note that a local closure of the triple-moment term is also possible by assuming a gradient-diffusion parameterization at the higher moment level,

$$\overline{w'w'c'} = -C_3 \tau \overline{w'w'} \frac{\partial \overline{w'c'}}{\partial z}, \quad (17)$$

where C_3 is another similarity constant. When this formulation for the triple moment is used in Eqs. (4) and (6), the resulting closure model is “prognostic” because it allows one to determine fluxes by their mean gradients. Moreover, this formulation is also consistent with the Lagrangian LNF in which the deviation from K theory applied to momentum or scalar fluxes is related to local sources or sinks inside the canopy ([Raupach 1989](#); [Siqueira et al. 2000](#); [Siqueira and Katul 2002](#); [Cava et al. 2006](#)). On the other hand, the nonlocal closure model given by Eqs. (15) and (16) is more “diagnostic” in nature, since ΔS_0 cannot be predicted beforehand but can be calculated on the basis of quadrant analysis from experimental data or simulation outputs, which encompasses the objective of this work. We use LES for turbulent flows in horizontally homogeneous forest canopies to explore this failure of K theory and its link to nonlocal organized eddy motion.

3. Simulations

The Parallelized LES Model (PALM; [Raasch and Schröter 2001](#); [Maronga et al. 2015](#)) is used to simulate flow through a horizontally homogeneous canopy. The representation of the canopy in the LES follows the standard distributed drag parameterization ([Shaw and Schumann 1992](#); [Watanabe 2004](#); [Patton et al. 2016](#)) by adding an additional term in the momentum budget equations as $F_{di} = -C_d a |\bar{u}| \bar{u}_i$, where a is a one-sided frontal plant area density, C_d is a dimensionless drag coefficient assumed to be 0.3 ([Katul et al. 2004](#); [Banerjee et al. 2013](#)), $|\bar{u}|$ is the resolved wind speed, and $|\bar{u}_i|$ is the resolved velocity component ($i = 1, 2, 3$; i.e., u , v , and w), that is, the overbar denotes here implicit averaging over a grid box in LES. The effect of the canopy on the sub-grid-scale (SGS) turbulence is accounted for by adding a sink term to the prognostic equation for the SGS turbulent kinetic energy e as $F_\varepsilon = -2C_d a |\bar{u}| e$. For closure of the SGS covariance terms, PALM uses a 1.5-order closure developed by [Deardorff \(1980\)](#) and modified by [Moeng and Wyngaard \(1988\)](#) and [Saiki et al. \(2000\)](#) that assumes a gradient-diffusion parameterization. The diffusivities associated with this gradient diffusion are parameterized using the SGS TKE and include a prognostic

equation for the SGS TKE. This SGS TKE scheme after [Deardorff \(1980\)](#) is deemed to be an improvement over the more traditional [Smagorinsky \(1963\)](#) parameterization because the SGS TKE allows for a much better estimation for the velocity scale corresponding to the sub-grid-scale fluctuations ([Maronga et al. 2015](#)). Further details of the LES model can be found in the literature and are not discussed here ([Shaw and Schumann 1992](#); [Watanabe 2004](#); [Maronga et al. 2015](#); [Patton et al. 2016](#)). Numbers of grid points in the x , y , and z directions are 320, 320, and 320, respectively, with grid resolutions of 7.81, 7.81, and 3.90 m in each direction. Each simulation is run for 10 000 s with a time step of 0.1 s, and the output of the first 6400 s is discarded to achieve computational equilibrium; that is, the profiles are quasi stationary when we perform the averaging for the data analysis during the final hour of the simulation. The canopy height h_c is taken as 35.0 m with a plant area index of 5.0, similar to the specification in a recent simulation study of [Dias-Junior et al. \(2015\)](#).

The simulation is driven by a geostrophic wind, which leads to a pressure gradient within the domain, and by the surface buoyancy flux, with a sensible and latent heat component. Our motivation to simulate a convective boundary layer is that we will analyze the correlation between temperature and vertical velocity, for which we set a source term for the temperature and moisture budgets. Hence, the boundary conditions at the bottom are Neumann for potential temperature and humidity but Dirichlet for the velocity (no slip). The lateral boundary conditions are periodic, with the horizontal extent of the domain about 5 times the boundary layer height, which is sufficient to capture the largest buoyant eddies. For potential temperature and

humidity, the kinematic sensible heat flux at the top of the canopy $\overline{w'T'_{hc}}$ is equal to 0.18 K m s^{-1} , and the latent heat flux at the surface $\overline{w'q'_s}$ is $1.0 \times 10^{-4} \text{ kg kg}^{-1}$. The canopy model assumes that inside the canopy there is an exponential decay of the radiation falling on top of the canopy, proportional to the downward cumulative leaf area index ([Shaw and Schumann 1992](#)). The additional heat flux within the canopy $Q_c(z)$ is then obtained from the vertical gradient of the radiation within the canopy:

$$Q_c(z) = \overline{w'T'_{hc}} \exp \left[-0.6 \int_z^{h_c} \text{LAD}(z) dz \right]. \quad (18)$$

We have chosen to model the vertical profile of the leaf area density with a beta distribution according to

$$\text{LAD}(z) = 12 \frac{\text{LAI}}{h_c} \left(\frac{z}{h_c} \right)^2 \left(1 - \frac{z}{h_c} \right). \quad (19)$$

The exponents of the beta distribution were chosen so as to obtain a crown-dense canopy as in [Dias-Junior et al. \(2015\)](#). The total LAI is equal to 5.

For the velocity, Monin–Obukhov similarity is applied within the lowest grid cell. The top boundary condition for the velocity is also Dirichlet, equal to the geostrophic wind:

$$(u_g, v_g) = (10.0 \text{ m s}^{-1}, 0.0 \text{ m s}^{-1}). \quad (20)$$

For potential temperature and humidity, the top boundary conditions are Neumann, such that the gradient of the initial gradient is maintained at the top of the domain. The domain is initialized with a potential temperature profile such that the top of the domain is well above the boundary layer height and a similar approach is used for the moisture:

$$T(z, 0) = 307.7 \text{ K} + 5.0 \times 10^{-2} Y(z - z_i + 20 \text{ m}) Y[-(z - z_i - 20 \text{ m})] (z - z_i + 20 \text{ m}) \text{ K m}^{-1} \\ + 2.5 \times 10^{-2} Y(z - z_i - 20 \text{ m}) (z - z_i - 20 \text{ m}) \text{ K m}^{-1} \quad \text{and} \quad (21)$$

$$q(z, 0) = 0.02 \text{ kg kg}^{-1} - Y(z - z_i + 20 \text{ m}) \\ \times Y[-(z - z_i - 20 \text{ m})] (z - z_i + 20 \text{ m}) \\ \times 4.38 \times 10^{-4} \text{ kg kg}^{-1} \text{ m}^{-1}, \quad (22)$$

where $Y(z)$ is the Heaviside function and $z_i = 500 \text{ m}$ is the boundary layer height at the start of the simulation. There is a capping inversion between 480 and 520 m with a local lapse rate of $5.0 \times 10^{-2} \text{ K m}^{-1}$, and there is a stable profile above with a smaller lapse rate of $2.5 \times 10^{-2} \text{ K m}^{-1}$.

4. Results and discussion

a. LES outputs

Before exploring the theory presented in [section 2](#), it is important to assess the output of the LES. Temporally and spatially averaged turbulent statistics are presented in [Fig. 1](#). The profiles match the LES profiles reported in [Dias-Junior et al. \(2015\)](#) qualitatively. The mean velocity profile U normalized by the friction velocity u_* calculated as $(-\overline{u'w'})^{1/2}$ at the canopy top shows the usual inflection point as it shifts from an

FIG. 1. Summary statistics of the LES simulation over the horizontally homogeneous canopy: (a) mean wind speed, (b) potential temperature, (c) (subgrid) TKE, (d) sensible heat flux, (e) momentum flux, (f) standard deviation of streamwise and vertical wind, (g) skewness of streamwise and vertical wind, and (h) efficiency of momentum transport.

exponential-type profile to a logarithmic law above the canopy top (Fig. 1a). The potential temperature θ decreases above the canopy top and is more or less constant inside the canopy (Fig. 1b). The TKE profile has a maximum at the canopy top and decreases both above and below the canopy (Fig. 1c). The sensible heat flux $\overline{w'\theta'}$ normalized by its value at the canopy top also decreases both above and inside the canopy (Fig. 1d). The Reynolds stress $\overline{u'w'}$ normalized by u_*^2 is attenuated inside the canopy as expected and remains almost constant (decreasing slowly) above the canopy (Fig. 1e). The standard deviation of the u and w velocity fluctuations (σ_u and σ_w) normalized by u_* are shown in Fig. 1f by a black dashed line and a blue solid line, respectively. As expected, the intensity of σ_u is higher than σ_w , and their trends are different; σ_u decreases with z above the canopy, and σ_w remains more uniform with height—consistent with observations in the surface layer (Banerjee and Katul 2013). Figure 1g shows the skewness of u and w defined as $Sk_u = \overline{u'u'w'}/\sigma_u^3$ and $Sk_w = \overline{w'w'w'}/\sigma_w^3$ by the dashed black line and the solid blue line, respectively. Consistent with the observations by several studies, (Baldocchi and Meyers 1988; Katul 1998; Finnigan 2000; Poggi et al. 2004b; Launiainen et al. 2007; Dias-Junior et al. 2015), nonzero skewness is observed, an indicator of heterogeneous non-Gaussian

turbulence both inside and above the canopy, even when the canopy is horizontally homogeneous. Inside the canopy, Sk_u is positive, and it is negative above the canopy; Sk_w has the opposite trend: it is negative inside the canopy and positive above the canopy. The two profiles cross over slightly above the canopy where $Sk_u = Sk_w = 0$. These different signs of nonzero skewness indicate the importance of sweep and ejections inside and above the canopy. Figure 1h plots the efficiency of momentum transport $-r_{wu} = -\overline{w'u'}/(\sigma_u\sigma_w)$. As observed, $-r_{wu}$ has its maximal value near the canopy top, and it decreases very fast inside the canopy, which is consistent with other studies as well (Raupach et al. 1996; Launiainen et al. 2007; Dupont and Brunet 2009; Dias-Junior et al. 2015). Hence, the LES results can be used to study the flux budget equations, failure of K theory, and the linkage to sweep–ejection cycles.

b. Evaluating K theory

Figure 2 allows us to evaluate K theory for the simulated flow through the canopy. The first two panels (momentum and scalar) show the Reynolds stress $\overline{u'w'}$ and the sensible heat flux $\overline{w'\theta'}$ obtained directly from the LES as black solid lines. The red dashed lines in the first and second panels show the gradient-diffusion

FIG. 2. Evaluating the validity of K theory: The LES output for the (left) momentum flux and (center) heat flux is compared with the components of the momentum and heat budgets, respectively, as well as the full budget from Eqs. (4) and (6). The budget for the scalar flux agrees well with the LES output; for the momentum flux, the budget overestimates the LES output in the canopy sublayer. (right) Different approaches for obtaining the relaxation time scale. Inside and far above the canopy, both the Rotta model and the Poggi model are off, but the Rotta model agrees well with the LES between 1 and 4 times the canopy height.

estimation of the $\overline{w'\theta'}$ flux, that is, only the first terms in Eqs. (4) and (6). The black open circles in the first two panels plot the triple-moment terms in the two equations [Eqs. (4) and (6)], respectively. In a similar way, the blue dashed lines in the first two panels show the buoyancy terms in the two equations [Eqs. (4) and (6)]. The full model including the buoyancy and triple-moment corrections—that is, the full rhs estimation of Eqs. (4) and (6)—is plotted as cyan dotted lines in the first two panels. The third panel, called normalized relaxation time scale, shows the relaxation time scale τ normalized by multiplying by u_*/h_c using different estimates as discussed in section 2a. The black solid line plots the $\tau u_*/h_c$ directly obtained from the LES. The blue dashed line used τ computed from the Poggi et al. (2006) model, and the red dash-dotted line uses τ computed from the Rotta model using Eq. (5).

A few interesting observations can be made from Fig. 2. Note that the τ computed from the three different models are different from each other. Although there is similarity between them above the canopy, they are very different inside the canopy, indicative of multiple choices of length and time scales in canopy sublayer turbulence (Katul and Chang 1999). In the

first two panels, however, we use only the Rotta estimation of τ from the scalar Eq. (5) and apply it to compute both $\overline{u'w'}$ and $\overline{w'\theta'}$. The full equation (the cyan line) predicts the LES output of $\overline{w'\theta'}$ but highly underestimates $\overline{u'w'}$. Hence, “one size (of τ) does not fit all,” and a different estimate of τ is necessary to predict $\overline{u'w'}$. Anyway, what is evident from the first two panels is that gradient diffusion alone is not sufficient as a model to estimate either the heat flux or the momentum flux but needs additional corrections by the buoyancy term and the triple-moment term, with the correct separate choice of relaxation time scale for both (momentum and scalar). The linkage between the triple moment and the sweep–ejection cycles as discussed in section 2b is discussed next.

c. Evaluating the link between triple moments and nonlocal motions

Figure 3 explores the link between the triple moments and the nonlocal sweep–ejection motions. The left panel shows the features of sweep–ejection motions for momentum, and the right panel does so for the scalar (sensible heat). The black lines in the left and right panels show the ΔS_0 computed using quadrant analysis from the LES data following Eq. (8) for momentum and

FIG. 3. Evaluating the link between triple moment and nonlocal motions for (left) momentum and (right) scalar: Positive ΔS_0 indicates sweep domination, and negative ΔS_0 indicates ejection domination. The CEM and ICEM offer good approximations for the momentum as well as scalar quadrant analyses. The wiggles in the CEM and ICEM for the scalar at large z arise because they first are computed locally before the final profile is obtained by horizontal averaging.

scalar, respectively. The red plus signs plot the CEM approximation for ΔS_0 given by Eq. (9). The blue open circles plot the ICEM approximation for ΔS_0 given by Eq. (14). As observed, both the CEM and ICEM approximations do a decent job of predicting the correct height variation of ΔS_0 , which is independently computed using quadrant analysis. The computation of the CEM and ICEM approximations to ΔS_0 makes use of turbulent data output restricted to the x - z plane. To obtain the profile, the turbulent data are then averaged in time and in the x direction. This procedure is the cause of the noise for $z > 5h_c$, resulting from the absence of additional averaging in the y direction, which can be performed for the profiles that are computed online. The fact that the ICEM predicts ΔS_0 well lends confidence to the linkage established between ΔS_0 and the triple moment $\overline{c'w'w'}$, as given by Eq. (14). Another important point to note is that, for both momentum and sensible heat flux, sweeps dominate inside the canopy, whereas the space above the canopy is dominated by ejection. This observation is also consistent with the outcome in Dias-Junior et al. (2015). Hence, the link between the shortcomings of K theory and the sweep-ejection cycles via the triple moment can be explored with sufficient confidence and is discussed next.

d. Connecting the failure of K theory to sweep-ejection cycles

Figure 4 (top panels) shows the triple moment calculated from the LES (black solid line) and its estimates using ΔS_0 computed from quadrant analysis (red dash-dotted line), ICEM (green dashed line), and CEM (blue dotted line) approximations for the (left panel) momentum (left panel) and scalar (right panel). Another estimation using Eq. (17) is also plotted using black open circles; it does a very poor job in estimating $\overline{w'w'u'}$ or $\overline{w'w'\theta'}$. In comparison, the quadrant-analysis, CEM, and ICEM estimates perform much better. In the bottom panels (left panel for momentum, and right panel for scalar), the momentum and sensible heat fluxes are plotted again, with their different estimates but with the triple moment parameterized using ΔS_0 as shown in the top panels. The estimate using K theory is shown by red dashed lines. The black open circles show the full estimate of the fluxes with the buoyancy and triple-moment correction, where the triple moment is parameterized using quadrant analysis (labeled QA in the figure key). The blue plus signs show the same full estimate but where the triple moment is parameterized using ICEM. To observe the effect of buoyancy, the full model with the triple moment parameterized using quadrant analysis but

FIG. 4. (top) The triple moments calculated for momentum and scalar from LES and estimated using different methods. (bottom) The momentum and scalar fluxes while the triple moment is closed with different methods, with and without buoyancy.

without buoyancy is plotted in cyan dash-dotted lines. The green dotted lines plot the full model with ICEM but without buoyancy. The same τ estimated from the Rotta model for the scalar has been used for both momentum and the sensible heat flux. As evident, the full model performs very well in predicting $w'\theta'$. To predict the momentum flux well, however, a different τ is needed, as we already remarked in section 4b. Furthermore, for the sensible heat flux, the performance of K theory is actually comparable to that of a truncated ICEM and quadrant analysis with the triple moment included but the buoyancy term omitted. This means that (at least for predicting the sensible heat flux), in contrast to the triple moments, the buoyancy term is the crucial term to improve K theory. For the buoyancy term, we have not established a clear connection to the sweep-ejection motions. Nevertheless, the most important physical insight that can be drawn from Fig. 4 is that it shows the importance of the nonlocal sweep-ejection motions if one wishes to overcome the shortcomings of K theory.

5. Conclusions

Flux-gradient turbulence modeling, or K theory, is found to be an inadequate modeling approach for canopy turbulence. Meanwhile, large-eddy simulation

has become a standard tool for investigating turbulent flows in vegetation canopies. Hence, in this work we study the failure of K theory in relation to sweep-ejection events by means of LES. Typical causes for K -theory failure are near-field effects, local imbalance between turbulence production and dissipation, and large-scale vertical transport by coherent eddies acting at the canopy scale. The large-scale transport that happens on the scale of the canopy height can be diagnosed by studying ejection-sweep cycles with a classical quadrant analysis.

Although flux-gradient modeling is inadequate, improved turbulence-modeling schemes for canopy turbulence are available in the literature. The flux budgets for stationary, horizontally homogeneous canopy turbulence can be reformulated by invoking Rotta's model, leading to expressions for the momentum and buoyancy fluxes as functions of the local gradients (as would be done by simple K theory) but augmented by a triple-moment term and a temperature covariance term for the sensible heat flux budget (or, respectively, a flux-divergence term in the momentum budget). At least the triple-moment term can be readily linked in function to the sweep-ejection cycle, as can be shown analytically by the cumulant expansion method.

The removal of the pressure correlation through Rotta's model introduces a relaxation time scale, for

FIG. A1. Evaluation of the Rotta model for momentum to obtain the relaxation time scale: (left) the pressure–velocity interaction, (left center) (minus) the velocity gradient term, (center right) the sum of both, yielding $C_R(\overline{w'u'})/\tau$, and (right) the normalized relaxation time scale obtained from the Rotta model for momentum.

which we investigate three approaches. It turns out that the time scale in the momentum budget needs a different prescription than the time scale in the sensible heat flux budget: *one size does not fit all*.

To connect the failure of K theory with ejection–sweep cycles, we have compared different calculation approaches for the triple moments for momentum and temperature. We clearly found that the approaches that include ejection–sweeps events, be it through quadrant analysis or (incomplete) cumulant expansion, approximate the LES results very well, in contrast to the gradient–diffusion approach. Hence, for predicting the triple moments, the sweep–ejection cycle is the necessary ingredient to improve K theory. For the buoyancy flux, however, the LES output also agrees well with full closure from quadrant analysis and ICEM but does not if the buoyancy is excluded in a truncated quadrant analysis or ICEM. Therefore, to describe also the second moments satisfactorily, the sweep–ejection cycle alone does not suffice: the buoyancy term needs to be taken into account.

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APPENDIX

Evaluating Relaxation Time Scale from the Rotta Model

As mentioned in the main text, the relaxation time scale obtained from the Rotta model for scalar has been used for both momentum and scalar fluxes. This was done on the basis of the assumption that the Rotta model for both scalar and momentum should yield the same relaxation time scale. However, it was found out that this choice of Rotta model is only able to capture the correct profile for scalar flux and is unable to capture the momentum flux profile. The purpose of using this

approach was to demonstrate that one choice of relaxation time scale does not fit both momentum and scalar. Whether a new formulation is necessary for relaxation time scale for the canopy sublayer is beyond the scope of the current work—we only intended to show that the standard formulation is accurate for scalar while being inaccurate for momentum.

Here, we present the confirmation that the τ from both Eqs. (3) and (5) are indeed equivalent. Figure A1 shows the two different terms in Eq. (3) needed to obtain τ . The left panel shows the pressure–velocity interaction term, and the left-center panel shows the term attached to velocity gradient. The right-center panel shows the sum of these two terms, and the right panel shows the computed τ for momentum. As observed, the computed τ here is very similar to the τ computed for the scalar in Fig. 2 in the paper. This confirms the assumption that the Rotta formulation yields the same relaxation time scale for both scalar and momentum. This choice does not capture the correct stress profile as obtained from the LES, however. This point raises an issue that was previously unknown in canopy turbulence, and in this work we only intend to raise this issue and present this observation. Future works will attempt to develop a modified Rotta model of momentum flux for canopy flows.

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