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# The mean wind and potential temperature flux profiles in convective boundary layers

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ABSTRACT: We develop innovative analytical expressions for the mean wind and potential temperature flux profiles in convective boundary layers (CBLs). CBLs are frequently observed during daytime as the Earth's surface is warmed by solar radiation. Therefore, their modeling is relevant for weather forecasting, climate modeling, and wind energy applications. For CBLs in the convective-roll dominated regime, the mean velocity and potential temperature in the bulk region of the mixed layer are approximately uniform. We propose an analytical expression for the normalized potential temperature flux profile as a function of height, using a perturbation method approach in which we employ the horizontally homogeneous and quasi-stationary characteristics of the surface and inversion layers. The velocity profile in the mixed layer and the entrainment zone is constructed based on insights obtained from the proposed potential temperature flux profile and the convective logarithmic friction law. Combining this with the well-known Monin-Obukhov similarity theory allows us to capture the velocity profile over the entire boundary layer height. The proposed profiles agree excellently with large-eddy simulation results over the range of  $-L/z_0 \in [3.6 \times 10^2, 0.7 \times 10^5]$ , where L is the Obukhov length and  $z_0$  is the roughness length.

### 1. Introduction

Convective boundary layers (CBLs) are frequently observed during daytime as the Earth's surface is warmed by solar radiation (Stull 1988). Due to their frequent occurrence, the fundamental understanding of CBLs is highly relevant to agriculture, architectural design, aviation, climate modeling, weather prediction, and wind energy applications, to name a few. The modern scientific literature on CBLs goes back over 100 years. Initially, the focus was on low-altitude measurements, and with the introduction of more advanced measurement techniques, the focus gradually shifted upwards. However, only after the introduction of large eddy simulations (LES) in the early seventies, it has become widely accepted that thermodynamic indicators are most suitable to identify the different CBL regions (LeMone et al. 2019). However, obtaining analytical profiles that describe the wind and potential temperature flux in the entire CBL has remained challenging due to the different flow physics in the various CBL regions.

The CBL can be subdivided into three layers (excluding the roughness sublayer), i.e. the surface layer, the mixed layer, and the entrainment zone (see figure 1). The surface layer is characterized by a superadiabatic potential temperature gradient and a strong wind shear, which is usually described by the Monin-Obukhov similarity theory (MOST, Monin and Obukhov 1954). According to the MOST the non-dimensional wind speed and potential temperature gradient profiles are universal functions of the dimensionless height z/L, where z is the height above the surface and L is the surface Obukhov length (Obukhov 1946; Monin and Obukhov 1954). Many studies have pointed out that the MOST does not explain all important surface-layer statistics under convective conditions (Panofsky et al. 1977; Khanna and Brasseur 1997; Johansson et al. 2001; McNaughton et al. 2007; Salesky and Anderson 2020; Cheng et al. 2021) or very stable conditions (Mahrt et al. 1998; Cheng et al. 2005). In particular, the normalized wind gradient  $\phi_m = (\kappa z/u_*)(\partial U/\partial z)$  depends both on z/L and  $z_i/L$  (Khanna and Brasseur 1997; Johansson et al. 2001), where  $z_i$  is the height of the inversion layer (see figure 1). Nevertheless, MOST is still widely used in numerical weather prediction and climate models (Salesky and Anderson 2020), and thus will be used in the theoretical analysis and numerical simulations of this study. MOST applies only to the surface layer, and for it to be applicable, the absolute value of the Obukhov length L must be smaller than the height of the surface layer. Therefore we only consider the CBL with  $-z_i/L \gg 1$ . In particular, we focus on the convective-roll dominant regime with  $-z_i/L \gtrsim 10$  (Salesky et al. 2017). Furthermore, we focus on dry and cloud-free CBLs to avoid complications due to physical processes like evaporation, precipitation, and cloud formation.

The mixed layer is characterized by intense vertical mixing caused by warm air thermals rising from the ground. Within the mixed layer, the magnitude of the mean velocity is much larger than the variations in the mean velocity. Thus, for applications where the mean velocity gradient is unimportant, the wind speed and potential temperature can be regarded as uniform (Kaimal et al. 1976; Salesky et al. 2017). This insight is incorporated in various CBL models (Lilly 1968; Deardorff 1973; Stull 1976; Deardorff 1979; Tennekes and Driedonks 1981; Garratt et al. 1982). The entrainment zone is characterized by entrainment of

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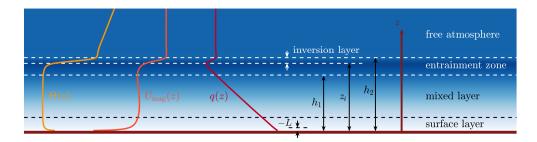


FIG. 1. Profiles of the potential temperature  $\Theta$ , wind speed  $U_{\text{mag}}$ , and potential temperature flux q in the CBL. The vertical lines with double arrows indicate different length scales in the CBL, namely, from left to right, the Obukhov length L, the lowest height where the potential temperature flux first reaches zero,  $h_1$ , the inversion layer height at which the potential temperature flux reaches its minimum value,  $z_i$ , and the height where the potential temperature flux first recovers zero,  $h_2$ . The background color indicates the magnitude of the potential temperature flux q(z) for case 2, see Table 1.

air from the free atmosphere. Deardorff et al. (1980) found in laboratory experiments that the ratio of the entrainment zone thickness to the depth of the mixing layer decreases asymptotically with increasing Richardson number Ri as follows  $(h_2 - h_1)/h_1 = 0.21 + 1.31/Ri$  (see figure 1 for the definitions of  $h_1$  and  $h_2$ ). This ratio is essential for developing entrainment models and has been studied extensively (Lilly 1968; Sullivan et al. 1998; Zilitinkevich et al. 2012; Haghshenas and Mellado 2019). The potential temperature flux profile decreases linearly with height and becomes negative in the entrainment zone. The entrainment flux ratio  $\Pi_m$ , which is defined as the ratio of the potential temperature flux at the inversion layer height to its value at the ground, turns out to be nearly constant, i.e.  $\Pi_m \approx -0.2$  (Stull 1976; Sorbjan 1996; Conzemius and Fedorovich 2006; Sun and Wang 2008; LeMone et al. 2019). Note that the inversion layer is the upper region of the entrainment zone in which the potential temperature flux increases steeply from its minimum value at  $z = z_i$  to zero at  $z = h_2$  (see figure 1).

The geostrophic wind  $(U_g, V_g)$  and the friction velocity  $u_*$  are usually connected through the well-known geostrophic drag law, which was initially derived for neutral boundary layers (Rossby and Montgomery 1935; Blackadar and Tennekes 1968; Tennekes and Lumley 1972) and later extended to include buoyancy effects (Zilitinkevich 1969). To include the effect of unsteadiness, Zilitinkevich and Deardorff (1974) and Arya (1975) proposed to replace the Ekman depth  $u_*/|f|$  in the geostrophic draw law, where f is the Coriolis parameter, with the time-dependent inversion layer height  $z_i$ . However, significant disparities were observed between the geostrophic drag law for CBLs and measurement data (Zilitinkevich 1975). Garratt et al. (1982) derived a relationship for the velocity defects in the mixed layer using a three-layer CBL model, which accounts for the effects of entrainment, baroclinity, advection, and local acceleration. In their formulation, the velocity defects are defined as the differences between the mixed-layer averaged winds and the geostrophic winds. They proposed a geostrophic drag law to relate the geostrophic winds and the friction velocity based on the assumption that the mean velocity at the top of the surface layer is equal to that in the mixed layer. In addition, an empirical stability function  $\psi_m$ , which may be inaccurate for large values of -z/L, is employed.

Recently, Tong and Ding (2020) analytically derived the convective logarithmic friction law from first principles. They identified three scaling layers for the CBL with  $-z_i/L \gg 1$ : the outer layer, the inner-outer layer, and the inner-inner layer. The characteristic length scales for these three layers are the inversion layer height  $z_i$ , the Obukhov length L, and the roughness length  $z_0$ , respectively. The mixed-layer mean velocity scale  $U_m$  and the geostrophic wind component  $V_g$  are the characteristic streamwise and spanwise velocity scales in the outer layer. The difference between the horizontally and temporally averaged velocity U(z) and  $U_m$  is the mixed-layer velocity-defect law, which has a velocity scale of  $u_*^2/w_* \ll U_m$  with  $w_*$  the convective velocity. This indicates that  $U_m$  is very close to the mean velocity U(z) in the mixed layer. For the innerouter layer they derived the surface-layer velocity-defect law, which states that the velocity defect  $U - U_m$  scales with  $u_*$ . The convective logarithmic friction law is derived from matching the law of the wall in the inner-inner layer with the velocity-defect law in the surface-layer. This exact leading-order result relates the friction velocity  $(u_*)$ to the mixed-layer velocity scale  $(U_m)$ . The difference between  $U_g$  and  $U_m$  scales as  $(u_*^2 w_e)/(f z_i)^2$ , where  $w_e$ is the entrainment velocity and  $V_g$  scales as  $-u_*^2/(fz_i)$ . Thus, up to non-dimensional coefficients, one can relate the geostrophic velocities  $(U_g, V_g)$  to  $u_*$ . As Tong and Ding (2020) do not consider the effects of the entrainment zone the velocity profiles are only valid for  $z/z_i < 0.4$ .

Various time-dependent models have been developed to explicitly account for entrainment processes at the top of CBLs (Troen and Mahrt 1986; Noh et al. 2003; Hong et al. 2006). For example, the counter-gradient transport method (Holtslag and Moeng 1991) and the eddy-diffusivity massflux approach (Siebesma et al. 2007; Li et al. 2021) are the Atmospheric Sciences widely used in coarse-resolution climate models. In general, the potential temperature is time-dependent (Lilly 1968) and the entrainment velocity can affect the mean wind speed in the mixed layer (Tong and Ding 2020). However, the velocity and potential temperature flux profiles are quasi-stationary, and therefore similarity theory can be employed to obtain analytical expressions for these profiles shapes (Zilitinkevich and Deardorff 1974; Arya 1975; Zilitinkevich et al. 1992).

In this study, we focus on the the derivation of analytical expressions for the mean velocity and potential temperature flux profiles in cloud-free CBLs. We use a perturbation method approach to construct an analytical expression for the normalized potential temperature flux profile as a function of height, taking into account the characteristics of both the surface layer and the capping inversion layer. The depth of the entrainment zone is connected to the convective logarithmic friction law to obtain analytical expressions for the velocity profile in the mixed layer and the entrainment zone. As remarked previously, the surface layer is still described by the MOST.

The organization of the paper is as follows. In Section 2 we obtain analytical expression for the potential temperature flux and wind profiles. In Section 3 we validate the proposed profiles against LES. The conclusions are given in Section 4.

## 2. Theory

### a. Potential temperature flux profile

The potential temperature flux profile provides a precise and convenient demarcation between the mixed layer and the entrainment zone of the CBL (Deardorff 1979; Deardorff et al. 1980). Figure 1 shows a definition of the various length scales in the CBL. Previous studies (Kaimal et al. 1976; Deardorff et al. 1980; Moeng and Sullivan 1994; Noh et al. 2003; Garcia and Mellado 2014; Haghshenas and Mellado 2019) showed that the potential temperature flux (including both the turbulent part and the diffusive part) in CBLs decreases linearly from its maximum value at the surface to a minimum value at  $z = z_i$ , and then increases steeply to zero in a narrow region  $z_i \le z \le h_2$  at the top of the boundary layer (figure 1). For typical CBLs the condition  $|dz_i/dt| \ll w_*$  holds, which implies that the boundary layer is quasi-stationary (Nieuwstadt et al. 2016, Section 7.6). Besides, the potential temperature flux q is fixed at the surface, and its value at the inversion layer height is nearly a constant fraction of the value at the ground  $q_w$ . Therefore, the normalized potential temperature flux  $q(z,t)/q_w$ only depends on the similarity variable  $\xi = z/h_2(t)$ , i.e.

where the form of  $\Pi$  remains to be determined. Using

$$q(z,t)/q_w = \Pi(\xi), \tag{1}$$

ordinary differential equation (ODE) for the determination of  $\Pi$ . However, it is important to emphasize that this does not mean  $\Pi$  is independent of time as the similarity variable  $\xi = z/h_2(t)$  is still time-dependent.

Under the assumption of horizontal homogeneity, the potential temperature equation reduces to

$$\frac{\partial \Theta}{\partial t} = -\frac{\partial q}{\partial z} = -\frac{q_w}{h_2} \Pi', \qquad (2)$$

where  $\Pi' = \partial \Pi / \partial \xi$ . In the mixed layer the potential temperature  $\Theta$  is almost spatially uniform and hence the lefthand side of Eq. (2) is independent of *z*. Therefore, the governing equation of the potential temperature flux in the mixed layer can be approximated as

$$-\Pi' = c_{\Pi},\tag{3}$$

where  $c_{\Pi}$  is the gradient of the normalized potential temperature flux in the mixed layer (see figure 1). In the mixed layer, it is well-known that the eddy-diffusivity approach cannot adequately describe the potential temperature flux as the gradient of the potential temperature nearly vanishes (Wyngaard 2010). In contrast, in the inversion layer the potential temperature gradient is dominant such that the potential temperature flux can be approximated by  $q = -v_{\theta} \partial \Theta / \partial z$ . Here  $v_{\theta} \propto |w_{\theta}| (h_2 - z_i)$  is the eddy diffusivity and  $w_e = dz_i/dt$  is the entrainment velocity. That the ratio  $h_2/z_i$  is approximately constant implies that  $\partial \xi / \partial t = -(z/h_2^2)(h_2/z_i)(dz_i/dt) \approx -w_e/z_i$ . From the zero-order jump model  $dz_i^2/dt$  is independent of time (Nieuwstadt et al. 2016, Section 7.6), such that  $v_{\theta}$ is approximately constant. Then, by taking the vertical derivative of Eq. (2), we obtain that

$$\epsilon \Pi'' - \Pi' = 0, \tag{4}$$

where  $\epsilon$  is a small dimensionless parameter,

$$\epsilon \equiv c \frac{h_2 - z_i}{h_2} \ll 1,\tag{5}$$

with  $c = (\nu_{\theta} z_i)/[-w_e h_2(h_2 - z_i)] = 1/2$  being an empirical constant that is determined by comparing the model profiles to the simulation results. This indicates that the parameter  $\epsilon$  represents the half thickness of the inversion layer normalized by the boundary layer depth (see figure 1). To get the potential temperature flux profile in the entire boundary layer, we combine Eqs. (3) and (4), which leads to the following second-order ODE for the potential temperature flux,

the potential temperature equation, we derive below an 
$$\epsilon \Pi'' - \Pi' = c_{\Pi} = \Pi(0) = 1$$
,  $\Pi(1) = 0$ . (6)

The solution of Eq. (6) reads

$$\Pi = 1 - c_{\Pi}\xi + (c_{\Pi} - 1)\frac{e^{\xi/\epsilon} - 1}{e^{1/\epsilon} - 1}, \quad 0 \le \xi \le 1.$$
(7)

Since  $\epsilon \ll 1$ , the value of  $\Pi$  in the bulk of the mixed layer can be approximated as

$$\Pi \approx 1 - c_{\Pi} \xi. \tag{8}$$

Similarly, since  $\Pi = 0$  at  $\xi = h_1/h_2$ , the slope  $c_{\Pi}$  reduces to

$$c_{\Pi} = h_2/h_1 > 1. \tag{9}$$

Therefore, the ratio of the entrainment zone thickness to the mixing layer depth is

$$R \equiv (h_2 - h_1)/h_1 = c_{\Pi} - 1 > 0.$$
 (10)

Deardorff et al. (1980) found in laboratory experiments that the value of *R* is between 0.2 and 0.4. Furthermore, the entrainment flux ratio  $\Pi_m$ , i.e. the minimum value of  $\Pi$ , can be approximated as

$$\Pi_m \approx 1 - c_{\Pi} (1 - 2\epsilon) \approx -(R - 2\epsilon). \tag{11}$$

Stull (1976) and Sorbjan (1996) found that  $-0.3 \le \Pi_m \le -0.1$ . This results is consistent with the LES results of Sullivan and Patton (2011) with  $\Pi_m \approx -0.2$ , the empirical results of Lenschow (1974) with  $\Pi_m = -0.1$ , and the direct numerical simulation results of Garcia and Mellado (2014) with  $\Pi_m \approx -0.12$ .

We note that the perturbation method approach to model the potential temperature flux profile was recently introduced by Liu et al. (2021b) for conventionally neutral atmospheric boundary layers where the surface potential temperature flux is always zero. However, it should be noted that in the CBLs under consideration, the surface is heated and thermal plumes are generated at the ground, resulting in significantly different turbulence generation mechanisms. The applicability of the perturbation method approach to model the strong inversion layer relies on its ability to capture the strong gradients in the inversion layer. Here we used the second-order ODE defined by Eq. (6) to model the potential temperature flux profile as our a posteriori tests confirm that this is sufficient to capture the inversion layer accurately. Higher-order terms could be incorporated, but this is not considered here to keep the obtained profiles relatively simple. An important observation is that the perturbation method approach is consistent with the finding of Garcia and Mellado (2014). They showed that the vertical structure of the entrainment zone is best described by two overlapping sublayers characterized by different length scales, namely the mean penetration depth of an overshooting thermal for the upper sublayer and the thickness of the CBL for the lower sublayer. Similarly, the second-order ODE, i.e. Eq. (6), indicates that there are two distinct length scales for the description of the entrainment zone (figure 1): one is the upper sublayer with  $z_i \le z \le h_2$ , where the gradient of potential temperature flux is proportional to  $-(q_w\Pi_m)/(2\epsilon h_2)$ , and the other is the lower sublayer with  $h_1 \le z \le z_i$ , where the gradient of potential temperature flux is proportional to  $(q_w\Pi_m)/(2\epsilon h_2)$ . Since  $\epsilon \ll 1$  the potential temperature flux varies much steeper in the upper sublayer than in the lower sublayer.

#### b. Wind profile

We consider MOST to describe the wind speed profile in the surface layer (Monin and Obukhov 1954). In surfacelayer coordinates, it states that the non-dimensional streamwise velocity gradient can be written as

$$\frac{\kappa z}{u_*} \frac{\mathrm{d}U}{\mathrm{d}z} = \phi_m\left(\frac{z}{L}\right),\tag{12}$$

where  $\phi_m$  is the dimensionless stability correction function and  $L = -u_*^3/(\kappa\beta q_w)$  is the Obukhov length with  $\beta$  the buoyancy parameter. By integrating Eq. (12), one can obtain the explicit formula for the streamwise velocity U,

$$\frac{\kappa U}{u_*} = \ln\left(\frac{z}{z_0}\right) - \psi_m\left(\frac{z}{L}\right). \tag{13}$$

Here  $\kappa = 0.4$  is the von Kármán constant,  $z_0$  is the roughness length, and

$$\psi_m = \int_{z_0/L}^{z/L} \frac{1 - \phi_m(\zeta)}{\zeta} \mathrm{d}\zeta \tag{14}$$

is the stability correction function for the momentum. We use the well-known Businger-Dyer expression (Paulson 1970; Businger et al. 1971; Dyer 1974; Brutsaert 1982)

$$\psi_m = \ln \frac{(1+x^2)(1+x)^2}{8} - 2\arctan x + \frac{\pi}{2}, \qquad (15)$$

with  $x = (1 - 16z/L)^{1/4}$  to model the stability correction function, but we note that other parameterizations exist (Katul et al. 2011). Note that  $\psi_m = 0$  for x = 1 (or  $L = \infty$ ), which reduces Eq. (13) to the classical logarithmic law for neutral boundary layers.

To model the wind profile U in the mixed layer and entrainment zone, we again employ a second-order ODE. In general, the detailed wind profile evolves when stability changes. However, the variations of the mean velocity are small compared to the magnitude of the mean velocity in the mixed layer when the stability parameter  $-z_i/L \ge 10$ (e.g. Salesky et al. 2017), which covers the range of stability conditions considered in this study. Thus, we can assume that the ODE is dominated by the U' = 0 term in most of the domain. Recently, Tong and Ding (2020) derived the convective logarithmic friction law from first principles, which connects the mixed-layer mean velocity scale  $U_m$ and the friction velocity  $u_*$  in the convective-roll dominant regime  $(-z_i/L \gg 1)$  as follows,

$$\frac{U_m}{u_*} = \frac{1}{\kappa} \ln\left(-\frac{L}{z_0}\right) - C,\tag{16}$$

where C = 1 is an empirical constant determined from our LES database (see below).

From the potential temperature flux profile modeling we learned that the ODE should have a second-order derivative term  $\epsilon U''$  to model the entrainment zone near the top of the boundary layer. The top boundary condition is given by the geostrophic wind component  $U_g$ . The lower boundary condition is given by equaling Eqs. (13) and (16), namely  $U(\xi_0) = U_m$ , since Tong and Ding (2020) showed that  $U_m$  is very close to U(z) in the mixed layer. Here  $\xi_0$  represents the height of the top of surface layer, which can be determined using Eqs. (13) and (16),

$$\ln\left(-\frac{h_2}{L}\xi_0\right) - \psi_m\left(\frac{h_2}{L}\xi_0\right) = -\kappa C \quad \Rightarrow \quad \xi_0 = \xi_0\left(\frac{h_2}{L}\right). \tag{17}$$

Because  $\epsilon \ll 1$ , the solution obtained from  $U(\xi_0) = U_m$  is almost the same as from  $U(0) = U_m$ , while the expression of the latter is much simpler. Therefore, we model the profile of the streamwise velocity U in the mixed layer and the entrainment zone as:

$$\epsilon U'' - U' = 0, \quad U(0) = U_m, \quad U(1) = U_g.$$
 (18)

The solution of Eq. (18) is

$$U = U_m + (U_g - U_m) \frac{e^{\xi/\epsilon} - 1}{e^{1/\epsilon} - 1}.$$
 (19)

We note that Eq. (19) is only valid in the mixed layer and entrainment zone as the wind speed in the surface layer is still modeled using the MOST. By combining Eqs. (13) and (19) and recalling that Eq. (13) increases monotonically as z increases, we obtain the following analytic description of the streamwise velocity profile U(z) for the entire CBL,

$$U = \begin{cases} \frac{u_*}{\kappa} \left[ \ln\left(\frac{z}{z_0}\right) - \psi_m\left(\frac{z}{L}\right) \right], & \xi \le \xi_0, \\ U_m + (U_g - U_m) \frac{e^{\xi/\epsilon} - 1}{e^{1/\epsilon} - 1}, & \xi_0 < \xi \le 1, \end{cases}$$
(20)

where  $\xi_0$  is given by Eq. (17). As remarked in Section 1 the surface layer profile contains two length scales, i.e.  $z_0$  for the inner-inner layer and the Obukhov length *L* for the inner-outer layer. Similarly, the velocity profile for the mixed layer and entrainment zone contains two length scales, i.e.  $z_i$  to describe the mixed layer and  $h_2 - z_i = 2\epsilon h_2$ to describe the upper sublayer of the entrainment zone.

This confirms the view presented by Tong and Ding (2020)that the entrainment zone has a different scaling than the surface and mixed layers, and can therefore be considered as another inner layer in the overall CBL problem. We note that the proposed analytical profile is empirical, similar to the MOST, and that the parameter  $\epsilon$  parameterizes the effect of various physical processes. We further note that  $U_m$  and  $u_*$  are related as given by Eq. (16), and that the difference  $U_g - U_m$  scales as  $(u_*^2 w_e)/(f z_i)^2$  (Tong and Ding 2020). Thus, Eq. (20) is predictive if the entrainment velocity  $w_e$  is given as an input parameter. To determine the value of  $w_e$ , one may need to revisit the entrainment processes at the top of CBLs (e.g. Garcia and Mellado 2014). In addition, the velocity predicted by Eq. (20) is continuous throughout the boundary layer and applicable for the considered ranges (see figure 5 below). However, its first derivative is discontinuous at the patching location  $\xi = \xi_0$ . This is a typical character of low-order models (Garratt et al. 1982). To capture the smooth transition, a high-order model is needed (Tong and Ding 2020). We leave these for future work.

To model the wind profile V in the the mixed layer and entrainment zone, we use a similar ODE as Eq. (18). The top boundary condition is given by the geostrophic wind component  $V_g$ . As the spanwise velocity V is small compared to the streamwise velocity U in the mixed layer (Tong and Ding 2020), the lower boundary condition is given by  $V(\xi_0) = V(0) = 0$ . Therefore, we model the profile of the spanwise velocity V in the entire boundary layer using

$$\epsilon V'' - V' = 0, \quad V(0) = 0, \quad V(1) = V_g.$$
 (21)

The solution of Eq. (21) is

$$V = V_g \frac{e^{\xi/\epsilon} - 1}{e^{1/\epsilon} - 1}.$$
(22)

Since  $V_g$  scales as  $-u_*^2/(fz_i)$  (e.g. Wyngaard 2010; Tong and Ding 2020), the geostrophic wind component  $V_g$  can be connected to  $u_*$ , up to a non-dimensional coefficient  $-V_g fz_i/u_*^2 = 0.66$ , which is determined from our LES database (see Table 1).

#### 3. Numerical validation

#### a. Numerical method and computational setup

We use LES to simulate the CBL flow over an infinite flat surface with homogeneous roughness. We integrate the spatially-filtered Navier-Stokes equations and the filtered transport equation for the potential temperature (Albertson 1996; Albertson and Parlange 1999; Gadde et al. 2021; Liu et al. 2021a,b; Liu and Stevens 2021). Molecular viscosity is neglected as the Reynolds number in the atmospheric boundary layer flow is very high, and we the Atmospheric Sciences use the advanced Lagrangian-averaging scale-dependent model to parameterize the sub-grid scale shear stress and potential temperature flux (Bou-Zeid et al. 2005; Stoll and Porté-Agel 2008). We note that the Lagrangian-averaging scale-dependent model has been extensively validated and widely used in the literature (Bou-Zeid et al. 2005; Stoll and Porté-Agel 2008; Calaf et al. 2010; Wu and Porté-Agel 2011; Zhang et al. 2019; Gadde et al. 2021).

Our code is an updated version of the one used by Albertson and Parlange (1999). The grid points are uniformly distributed, and the computational planes for horizontal and vertical velocities are staggered in the vertical direction. The first vertical velocity grid plane is located at the ground. The first gridpoint for the horizontal velocity components and the potential temperature is located at half a grid distance above the ground. We use a secondorder finite difference method in the vertical direction and a pseudo-spectral discretization in the horizontal directions. Time integration is performed using the secondorder Adams-Bashforth method. The projection method is used to enforce the divergence-free condition. At the top boundary, we impose a constant potential temperature lapse rate, zero vertical velocity, and zero shear stress boundary condition. At the bottom boundary, we employ the classical wall stress and potential temperature flux formulations based on the MOST (Moeng 1984; Bou-Zeid et al. 2005; Stoll and Porté-Agel 2008; Gadde et al. 2021).

We perform eleven LES to verify the validity of the derived wind speed and potential temperature flux profiles for CBLs. The computational domain is  $5 \text{km} \times 5 \text{km} \times 2 \text{km}$ and the grid resolution is  $256 \times 256 \times 256$ . Due to large computational expense, only several external parameters are varied in the simulations. The flow is driven by the geostrophic wind of  $G = \sqrt{U_g^2 + V_g^2} = 10$  m/s, the buoyancy parameter is  $\beta = 0.0325 \,\mathrm{m}/(\mathrm{s}^2 \cdot \mathrm{K})$ , and the Coriolis parameter is  $f = 1 \times 10^{-4}$  rad/s (Moeng and Sullivan 1994; Abkar and Moin 2017; Gadde et al. 2021). To ensure the CBLs are in the convective-roll dominant regime with  $-z_i/L \gtrsim 10$ , the surface potential temperature flux is set to  $q_w = 0.12 \sim 0.24 \,\mathrm{K} \cdot \mathrm{m/s}$ . Note that the convective logarithmic friction law (Eq. (16)) is derived very recently by Tong and Ding (2020) and tested only in a relatively narrow range of  $-L/z_0$ , namely  $-L/z_0 \in [2.5 \times 10^2, 1.5 \times 10^3]$ . To evaluate the performance of this law in much wider range, i.e.  $-L/z_0 \in [3.6 \times 10^2, 0.7 \times 10^5]$ , the roughness length is varied between  $z_0 = 0.0002$  m and  $z_0 = 0.16$  m, where the lower bound of  $z_0$  is set to a representative value of the sea surface (Wieringa et al. 2001). The vertical potential temperature gradient is varied between  $\Gamma = 1$  K/km and  $\Gamma = 9$  K/km to capture the relevant range observed in atmospheric measurements (Sorbjan 1996). The velocity field is initialized with the geostrophic wind G = 10 m/s. The initial potential temperature is 300 K up to 937 m and increases with 8 K in the next 126 m above. Above 1063 m the Published by Journal of

constant vertical derivative of the potential temperature  $\Gamma$  is specified. The simulations are run for about 25 large-eddy turnover times  $T = z_i/w_*$ , where  $w_* = (\beta q_w z_i)^{1/3}$  is the convective velocity scale, and the statistics are computed from the time interval of 12*T* to 25*T* when the boundary layer is quasi-stationary (Ding and Tong 2021). We note that inertial oscillation develops as the flow is initialized with a profile in geostrophic equilibrium (Schröter et al. 2013). However, it should have only negligible effect on the simulated statistics since the typical large-eddy turnover time  $T \approx 10$  mins is two order smaller than the natural inertial periodicity  $2\pi/f \approx 17.5$  h.

A summary of all simulated cases is presented in Table 1. Note that the cases in Table 1 are arranged such that the value of  $-L/z_0$  increases monotonically. Furthermore, we note that case 2 has been validated against atmospheric observations, and the simulation results obtained using different sub-grid scale models and grid resolutions is very similar (Gadde et al. 2021). To show the simulated results are independent of the computational domain size, we have performed an additional simulation for case 2 in a larger computational domain  $(12 \text{km} \times 6 \text{km} \times 2 \text{km})$  on a mesh with  $600 \times 300 \times 240$  nodes such that the grid spacings are nearly identical. Figure 2 shows the simulated wind speed and potential temperature flux profiles for case 2. The good agreement between the results obtained with different computational domain size confirms that the simulated results are independent of the computational domain size.

## b. Validation of analytical profiles

Figure 3 shows that with increasing height the normalized potential temperature flux profile  $q/q_w$  first decreases linearly from unity at the surface to a minimum at  $z_i/h_2 = 1 - 2\epsilon$ , before it rapidly increases to zero in the inversion layer  $(1 - 2\epsilon \le z/h_2 \le 1)$ . The normalized thickness of the inversion layer, which is parameterized by  $\epsilon$ , is expected to depend on the Richardson number (Deardorff et al. 1980), potential temperature gradient (Sorbjan 1996), and wind shear (Conzemius and Fedorovich 2006). However, we find that for the parameter range under consideration, the variation in the normalized thickness of the inversion layer is limited (see Table 1). Therefore, we use a fixed representative value  $\epsilon = 0.044$  to model the potential temperature flux profile, and the figure confirms that this ensures that the potential temperature flux profile obtained from the model agrees excellently with all available simulation data, which validates the chosen approach. To further confirm the validity of the potential temperature flux profile, we also compare our results in figure 3 with previous LES from Mason (1989), Sorbjan (1996), and Abkar and Moin (2017), the direct numerical simulations data by Garcia and Mellado (2014), and the empirical models by Lenschow (1974) and Noh et al. (2003). Clearly, the model predictions agree well with these previous studies.

TABLE 1. Summary of all simulated cases. Here  $\Gamma = \partial \Theta / \partial z$  is the vertical derivative of the mean potential temperature in the free atmosphere,  $q_w$  is the surface potential temperature flux,  $z_0$  is the roughness length,  $u_*$  is the friction velocity,  $U_m$  is the wind speed in the mixed layer, L is the Obukhov length,  $z_i$  is the inversion layer height,  $|V_g|$  is the magnitude of the spanwise geostrophic wind,  $\epsilon$  and  $c_{\Pi}$  are dimensionless parameters calculated by Eqs. (5) and (9), respectively, and  $Ri = \beta \Delta \Theta z_i / w_*^2$  is the Richardson number, where  $\Delta \Theta = \Theta(h_2) - \Theta(h_1)$  is the potential temperature difference across the entrainment zone and  $w_* = (\beta q_w z_i)^{1/3}$  is the convective velocity.

Case	$\Gamma$ (K/km)	$q_w \; (\mathrm{K} \cdot \mathrm{m/s})$	$z_0$ (m)	$u_*$ (m/s)	$U_m$ (m/s)	$ V_g $ (m/s)	$\epsilon$	$c_{\Pi}$	Ri	$-z_i/L$	$-L/z_{0}$
1	9	0.24	0.16	0.562	7.60	2.00	0.044	1.32	56.1	19.2	$3.6 \times 10^2$
2	3	0.24	0.16	0.563	7.59	1.87	0.052	1.34	51.0	19.1	$3.6 \times 10^2$
3	1	0.24	0.16	0.562	7.59	1.84	0.055	1.34	47.9	19.2	$3.6 \times 10^2$
4	3	0.12	0.16	0.533	7.70	2.20	0.046	1.34	94.2	11.0	$0.6 \times 10^3$
5	3	0.24	0.016	0.463	8.44	1.17	0.050	1.33	51.0	34.5	$2.0\times10^3$
6	3	0.20	0.02	0.468	8.36	1.32	0.046	1.31	59.6	27.5	$2.0 \times 10^3$
7	3	0.12	0.016	0.444	8.45	1.43	0.038	1.31	91.5	19.0	$3.5 \times 10^3$
8	3	0.20	0.002	0.392	8.93	0.86	0.033	1.28	55.5	47.3	$1.2 \times 10^4$
9	3	0.24	0.0016	0.389	8.94	0.75	0.044	1.30	50.4	58.3	$1.2 \times 10^4$
10	3	0.12	0.0016	0.375	8.94	0.88	0.036	1.30	93.9	31.6	$2.1 \times 10^4$
11	3	0.20	0.0002	0.334	9.24	0.57	0.041	1.30	58.6	75.8	$0.7 \times 10^5$

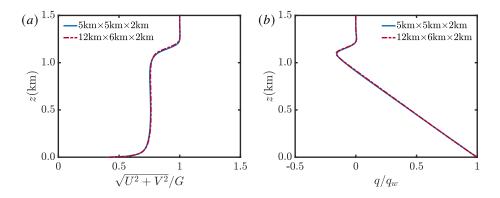


Fig. 2. The comparison of simulated (a) normalized wind speed  $\sqrt{U^2 + V^2}/G$  and (b) normalized potential temperature flux  $q/q_w$  profiles for case 2 (see Table 1) with different computational domain sizes.

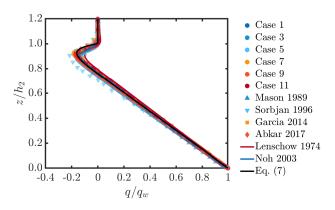


FIG. 3. Vertical profile of normalized potential temperature flux  $q/q_w$ . Circles: LES data (Table 1); up-triangle: LES data of Mason (1989); down-triangle: LES data of Sorbjan (1996); square: direct numerical simulations data of Garcia and Mellado (2014); diamond: LES data of Abkar and Moin (2017); red line: prediction given by Lenschow (1974); blue line: prediction given by Noh et al. (2003); black line: prediction given by Eq. (7) with  $\epsilon = 0.044$  and  $c_{\Pi} = 1.32$ . The figure shows that the proposed model captures the simulation trends very well.

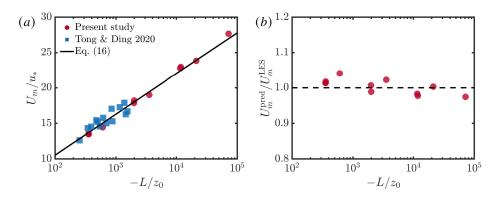


FIG. 4. The dependence of (a) the normalized mixed-layer mean velocity scale  $U_m/u_*$  and (b) the ratio of the predicted and simulated mixed-layer mean velocity scale  $U_m^{pred}/U_m^{LES}$  against the normalized Obukhov length  $-L/z_0$ . Circles: LES data (Table 1); squares: LES data of Tong and Ding (2020); solid line: prediction given by Eq. (16) with C = 1 determined using a fit to the present simulation data.

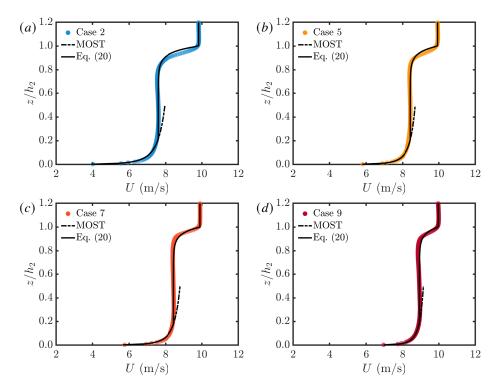


FIG. 5. Vertical profile of the mean streamwise velocity U. Filled circles: LES data (Table 1); dashed line: prediction given by Eq. (20) with  $\epsilon = 0.044$ . The prediction by the MOST is plotted outside the surface layer region to demonstrate the difference with the new profile.

In figure 4(a) we compare the wind speed in the bulk of the mixed layer  $(0.4 \le z/h_2 \le 0.6)$  against the normalized Obukhov length  $-L/z_0$  with results from Tong and Ding (2020). The figure shows that our simulations convincingly confirm the validity of the convective logarithmic friction law for the wind speed (Eq. (16) with C = 1) over a much wider range of  $-L/z_0 \in [3.6 \times 10^2, 0.7 \times 10^5]$  than previously considered  $(-L/z_0 \in [2.5 \times 10^2, 1.5 \times 10^3])$ . To further confirm the convective logarithmic friction law, figure 4(b) shows the ratio of the predicted and simulated mixed-layer mean velocity scale  $U_m^{\text{pred}}/U_m^{\text{LES}}$  against the normalized Obukhov length  $-L/z_0$ . The figure shows that the predicted value is within 5% of the simulation result for all considered cases.

In figure 5 we compare the vertical profile of the mean streamwise velocity U for four typical cases with different surface potential temperature flux and roughness length with the simulation results. The filled symbols are the her Atmospheric Sciences

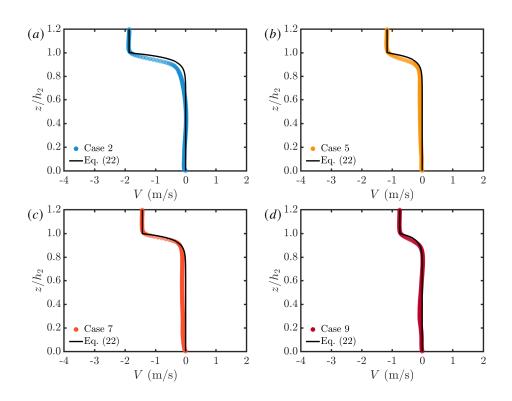


Fig. 6. Vertical profile of the mean spanwise velocity V. Filled circles: LES data (Table 1); solid line: prediction given by Eq. (22) with  $\epsilon = 0.044$ .

present LES data, the dashed line is the theoretical prediction given by the MOST, and the solid line is the prediction given by Eq. (20) with  $\epsilon = 0.044$ . The figure shows that the MOST accurately captures the surface layer's wind profile (lowest 20% of the boundary layer). However, in the mixed layer, the prediction of the MOST deviates significantly from the LES data. In particular, the discrepancy from the MOST increases as the surface potential temperature flux  $q_w$  decreases (figure 5b,c) or the roughness length  $z_0$  increases (figure 5a,d). Therefore, MOST is seldom used to specify wind profiles outside of the surface layer. Figure 5 shows that the proposed wind profile given by Eq. (20)accurately captures the velocity profile throughout the entire boundary layer. This excellent agreement confirms the validity of our proposed wind profile of Eq. (20) for atmospheric boundary layers in the range of studied parameters.

Figure 6 shows the corresponding profiles of the mean spanwise velocity *V*. The filled symbols are the present LES data and the solid line is the prediction given by Eq. (22) with  $\epsilon = 0.044$ . Overall, the agreement between the proposed wind profile given by Eq. (22) and the LES data is reasonably good in the entire boundary layer. This agreement confirms the validity of our proposed wind profile of Eq. (22) for CBLs in the range of studied parameters (i.e.  $-L/z_0 \in [3.6 \times 10^2, 0.7 \times 10^5]$ ). We note that the figure confirms that the spanwise velocity *V* is much smaller than the streamwise velocity  $U_p$ . The figure also indicates

that the magnitude of the geostrophic wind component  $|V_g|$  increases as the surface potential temperature flux  $q_w$  decreases (figure 6b,c) or the roughness length  $z_0$  increases (figure 6a,d).

#### 4. Conclusions

This work uses a perturbation method approach in conjuncture with the convective logarithmic friction law and the Monin-Obukhov similarity theory to develop analytical expressions of the wind and potential temperature flux profiles in convective atmospheric boundary layers. The validity of the proposed wind (given by Eqs. (20) and (22)) and potential temperature flux profiles (given by Eq. (7)) has been confirmed by their excellent agreement with largeeddy simulations results for atmospheric boundary layers in the convective-roll dominant regime with  $-z_i/L \gtrsim 10$ , where L is the Obukhov length and  $z_i$  the inversion layer height. Furthermore, our simulations confirm that the convective logarithmic friction law of Eq. (16), which was originally proposed by Tong and Ding (2020) for the mixed-layer mean velocity scale, is valid for an extensive range of  $-L/z_0$ , namely  $-L/z_0 \in [3.6 \times 10^2, 0.7 \times 10^5]$ , where  $z_0$  is the surface roughness length. Since accurate capturing the coupling between meso and microscale processes is a long-standing challenge in numerical weather predictions (Wyngaard 2004; Larsén et al. 2018; Veers et al. 2019), the proposed analytical profiles may be relevant for climate modeling and weather forecasting to better understand the effect of convective atmospheric boundary layers on, for example, wind farms. Possible future work will involve investigating models to predict the entrainment velocity at the top of CBLs and developing a high-order model that can capture the transition between the entrainment zone and free atmosphere. The latter may require a formal asymptotic series expansion of the governing equations, allowing for the separation into a time-dependent and steady-state problem at different orders.

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*Data availability statement.* The data that support the findings of this study are available from the corresponding author upon reasonable request.

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