# An Eddy Diffusivity–Mass Flux Approach to the Vertical Transport of Turbulent Kinetic Energy in Convective Boundary Layers

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ABSTRACT

In this study a new approach to the vertical transport of the turbulent kinetic energy (TKE) is proposed. The principal idea behind the new parameterization is that organized updrafts or convective plumes play an important role in transferring TKE vertically within convectively driven boundary layers. The parameterization is derived by applying an updraft environment decomposition to the vertical velocity triple correlation term in the TKE prognostic equation. The additional mass flux (MF) term that results from this decomposition closely resembles the features of the TKE transport diagnosed from the large-eddy simulation (LES) and accounts for 97% of the LES-diagnosed transport when the updraft fraction is set to 0.13. Another advantage of the MF term is that it is a function of the updraft vertical velocity and can be readily calculated using already existing parameterization. The new MF approach, combined with several eddy diffusivity (ED) formulations, is implemented into a simplified 1D TKE prognostic model. The 1D model results, compared against LES simulations of dry convective boundary layers, show substantial improvement in representing the vertical structure of TKE. The new combined ED–MF parameterization, as well as the MF term alone, surpasses in accuracy the ED parameterizations. The proposed TKE transport parameterization shows large potential of improving TKE simulations in mesoscale and global circulation models.

## 1. Introduction

Vertical turbulent fluxes of heat, humidity, and momentum are key elements in numerical models of planetary boundary layers. These fluxes are usually approximated using an eddy diffusivity (ED) approach, where vertical fluxes are assumed to be proportional to the local gradient of the mean profiles. A proportionality function, referred to as a $K$ or ED coefficient, is parameterized using formulations of various levels of complexity and physical sophistication (e.g., Holt and Raman 1988; Stull 1988; Wyngaard 1992). Higher-order closures, such as those based on the turbulent kinetic energy (TKE), are often more accurate in simulating various boundary layer scenarios than less sophisticated first-order closures (e.g., Mellor and Yamada 1982; Holt and Raman 1988; Alapaty et al. 1997; Lenderink and Holtslag 2000; Cuxart et al. 2006). For this reason they are becoming more popular in mesoscale and global atmospheric models. The success of higher-order schemes, however, relates directly to the accuracy of TKE simulations.

The ED approach has been fairly successful in a number of atmospheric conditions. It has, however, some structural limitations that hamper its performance in convective boundary layers (CBLs) or in neutrally stratified conditions, where the gradients of average profiles are close to zero. To address these issues the eddy diffusivity–mass flux (EDMF) framework has been developed (Siebesma and Teixeira 2000; Siebesma et al. 2007). It incorporates a nonlocal vertical turbulent transport of scalar variables, carried out by strong thermals or convective plumes that are common in CBLs. Accordingly, EDMF schemes inherit all benefits of the ED approach and further extend it with the nonlocal transport contribution that improves simulations of neutral and slightly stable atmospheric conditions associated with convective situations. The addition of the mass flux (MF) term has enabled a better coupling between dry convection and clouds and has improved simulations of potential temperature, humidity, and pollutant concentration (Teixeira and Siebesma 2000; Soares et al. 2004; Angevine 2005; Hurley 2007; Siebesma et al.

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2007; Soares et al. 2007; Neggers et al. 2009; Neggers 2009; Angevine et al. 2010).

Some of the EDMF schemes developed to date use a TKE closure to parameterize the ED coefficient (Soares et al. 2004; Angevine 2005; Angevine et al. 2010). A recent study by Witek et al. (2011) couples both ED and MF with a TKE closure. However, most of these parameterizations use only an ED approach to represent the vertical transport of TKE. This can lead to errors in simulating the TKE structure, especially in convectively driven boundary layers. The presence of strong, organized updrafts with high vertical velocities suggests a highly nonlocal redistribution of TKE. Updrafts themselves constitute a large part of TKE and they often extend through the entire depth of the CBL. Angevine et al. (2010) suggested that EDMF schemes based on TKE tend to dampen TKE above the middle of the boundary layer, primarily because of the negative buoyancy flux caused by slightly stable temperature profiles. Witek et al. (2011) argue that the ED transport of TKE leads to TKE underestimation in the upper parts of the CBL. Also, the relatively constant values of TKE in the mixed layer, as suggested by large-eddy simulation (LES) results, cannot be accurately resolved using only an ED parameterization. These facts point to the need for a nonlocal TKE transport parameterization, which could be employed in a similar fashion to that of the EDMF framework. In the present study we address this issue and propose a MF parameterization of vertical transport of TKE that, along with ED, forms an EDMF framework for TKE.

An alternative approach to the MF transport of turbulent energy was recently proposed by Angevine et al. (2010). Their scheme is based on the total turbulent energy, rather than TKE, which eliminates the problem of negative buoyancy in stably stratified conditions. Their approach for the MF vertical transport is similar to that used for scalar variables and is based on the difference in total turbulent energy between the updrafts and environment. However, they do not elaborate on the details of their formulation or investigate characteristics of their MF term. It also remains uncertain how their MF transport of total turbulent energy contributes to the overall performance of the scheme.

The paper is organized as follows. Section 2 describes LES results of the dry CBL cases investigated here. The EDMF parameterization for the TKE vertical transport is introduced in section 3. Additionally, some features of the parameterization are analyzed based on LES data. In section 4 a simplified one-dimensional (1D) model for TKE prognostic equation is developed. Results of this model, compared against LES, are used to verify the performance of the new parameterization. A summary and some conclusions follow in section 5.

## 2. LES simulations

The LES code used in this study is a modified version of the University of California, Los Angeles (UCLA)-LES (Stevens et al. 2005; Stevens and Seifert 2008; Matheou et al. 2011). The Favre-filtered (density-weighted) Navier–Stokes equations, written in the anelastic form (Ogura and Phillips 1962; Vallis 2006), are numerically integrated. The constant-coefficient Smagorinsky LES–subgrid-scale model (Smagorinsky 1963; Lesieur and Metais 1996) with Lilly's (1962) stability correction is used for turbulent momentum, temperature, and humidity transport. The Smagorinsky coefficient is set to $C_S = 0.23$. Scalar eddy diffusivities are assumed proportional to the momentum eddy diffusivity with a turbulent Prandtl number $\mathrm{Pr}_t = 1/3$. The discrete equations are integrated on a staggered mesh using fully conservative second-order accurate centered differences (Harlow and Welch 1965; Morinishi et al. 1998). Time integration is accomplished by a low-storage third-order Runge–Kutta method (Spalart et al. 1991). The time step is variable and is adjusted to maintain a constant Courant–Friedrichs–Lewy number of 0.3.

A series of four LES runs are performed with various surface sensible heat fluxes $\overline{w'\theta'}^s$ equal to 0.03, 0.06, 0.09, and 0.12 K m s$^{-1}$ (equivalent to approximately 30, 60, 90, and 120 W m$^{-2}$). Initial conditions are based on the profiles established by Nieuwstadt et al. (1992), which can be summarized by

$$\theta = 300\,\mathrm{K}, \quad \partial q/\partial z = -3.7\times 10^{-4}\,\mathrm{km}^{-1}, \quad 0 < z < 1350\ \mathrm{m},$$

$$\partial\theta/\partial z = 2\,\mathrm{K\,km}^{-1}, \quad \partial q/\partial z = -9.4\times 10^{-4}\,\mathrm{km}^{-1}, \quad z > 1350\ \mathrm{m}.$$

The surface humidity flux is kept constant at $\overline{w'q'}^s = 2.5\times 10^{-5}$ m s$^{-1}$. The surface pressure is set to $p_s = 1000$ hPa. The free convection conditions are assured by setting initial mean wind speed profile as $(u_0, v_0) = (0.01, 0)$ m s$^{-1}$. The LES simulations are performed on a domain with a uniform grid spacing of $\Delta x = \Delta y = \Delta z = 20$ m. The domain size is $8 \times 8$ km$^2$ in the horizontal, whereas in the vertical 4 and 5 km are used for the simulations with surface heat fluxes of (0.03, 0.06) and (0.09, 0.12) K m s$^{-1}$, respectively. Model results are output every 10 min.

Figure 1 shows normalized TKE and TKE budget terms (solid, dashed, and dashed–dotted black lines) obtained from the four LES simulations and averaged between the second and eighth simulation hour. The buoyancy source term $\overline{w'\theta_v'}(g/\overline{\theta}_v)$ and the transport term $-\partial\overline{w'e'}/\partial z - \partial\overline{w'p'}/\partial z$ are derived from the LES output.

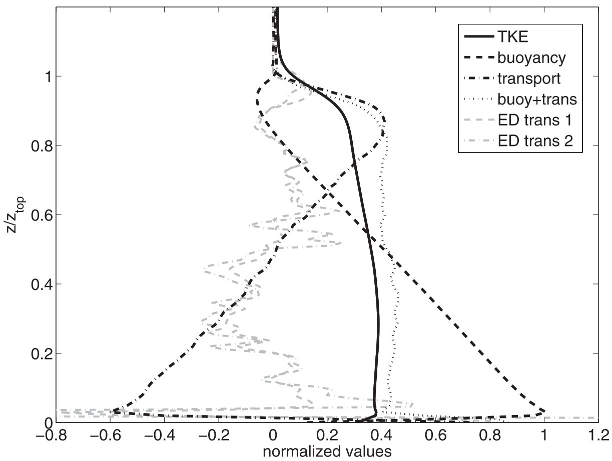


FIG. 1. Normalized TKE and TKE budget terms, averaged over LES results from 2 to 8 h. The gray dashed (ED transport 1) and dashed–dotted (ED transport 2) lines represent estimated eddy-diffusivity transport terms obtained using the TKE profile and two different $K$-coefficient parameterizations described in section 3.

Normalization of TKE is obtained by dividing by $w_*^2$, where $w_* = (g/T_v\overline{w'\theta_v'})_s^{1/3}$ is the convective velocity scale. The buoyancy and transport terms are normalized using $z_{\mathrm{top}}/w_*^3$, where $z_{\mathrm{top}}$ is the boundary layer height defined as the level of the maximum gradient of potential temperature (e.g., Siebesma et al. 2007).

The normalized TKE budget profiles exhibit a typical structure found in the CBL (e.g., Nieuwstadt et al. 1992). TKE is driven by the surface heating and resulting buoyant instabilities and transported upward by vertical velocity fluctuations. The turbulent transport is negative in the lower half of the CBL, being a local loss term, and positive in the upper half, contributing to the local TKE production. Integrated over the whole CBL, becomes zero. The sum of the buoyancy and transport terms, shown in Fig. 1 as the black dotted line, is almost constant within the CBL and decreases to zero at the inversion. The profile of TKE is also relatively constant with height, indicating that the TKE dissipation (not shown) scales directly with TKE. This suggests the form of a dissipation length scale, presented in section 4.

The average TKE profile from Fig. 1 can be used to assess the TKE transport as projected by different ED parameterizations, according to the formula $(\partial/\partial z)(K\,\partial e/\partial z)$, where $K$ is an ED coefficient and $e$ is the TKE. To estimate the ED transport terms, two different $K$ parameterizations ($K_1$ and $K_3$ in Table 1), combined with the conditions at the end of the LES simulation with surface flux 0.06 K m s$^{-1}$, are used. Results of the estimated ED transport are plotted in Fig. 1 as the gray dashed and dashed–dotted lines. Such a straightforward approach, even though highly simplified, reveals substantial difficulties of the ED parameterization in representing the TKE transport in CBLs. In particular, our simple test suggests that the TKE structure such as that presented in Fig. 1 is difficult to achieve using a classical ED formulation. Alternative approaches are required to address this problem. One such idea, which combines the ED and MF concepts, is introduced in the following section.

## 3. Basic concept of the eddy diffusivity/mass flux transport of TKE

The TKE prognostic equation can be written as (e.g., Stull 1988)

$$\frac{\partial e}{\partial t} = \frac{g}{\overline{\theta}_v}\overline{w'\theta_v'} - \frac{\partial \overline{w'e}}{\partial z} - \frac{1}{\rho}\frac{\partial \overline{w'p'}}{\partial z} - \varepsilon - \overline{u'w'}\frac{\partial \overline{u}}{\partial z} - \overline{v'w'}\frac{\partial \overline{v}}{\partial z}, \tag{1}$$

where the first term on the right-hand side (rhs) represents the buoyancy production, the second and third term represent the transport, $\varepsilon$ is the TKE dissipation, and the last two terms represent the shear production. The vertical transport by turbulent motions can be further split into

$$\frac{\partial \overline{w'e}}{\partial z} = \frac{1}{2}\left(\frac{\partial \overline{w'u'^2}}{\partial z} + \frac{\partial \overline{w'v'^2}}{\partial z} + \frac{\partial \overline{w'w'^2}}{\partial z}\right). \tag{2}$$

In CBLs the vertical motions can have large velocities and can be organized into localized ascending plumes. This suggests that an updraft environment decomposition can be applied to the vertical velocity triple correlations.

TABLE 1. Overview of the diffusion coefficient parameterizations used in this study. For a full description see the appendix.

| | $K_1$ | $K_2$ | $K_3$ |
|---|---|---|---|
| Expression and references | $K_1 = K_1\left(\frac{z}{z_{\mathrm{top}}}, u_*, w_*\right)$ (Holtslag 1998) | $K_2 = l_2 S_h \sqrt{e}$ (Bretherton and Park 2009) | $K_3 = a_3 l_3 \sqrt{e}$ (Witek et al. 2011; Galperin et al. 1988) |
| Surface layer scaling | Prescribed | $kz$ | $kzf(L)$ |
| Static stability scaling | Prescribed | Embedded in $S_h$<br>$S_h = S_h(N^2, l_2, e)$ | Embedded in $l_3$<br>$l_3 = \min[l_3, g(N, e)]$ |

A similar approach has been already successfully applied to the vertical fluxes of scalar variables in EDMF parameterizations. Following Randall et al. (1992) and Siebesma et al. (2007) gives

$$\overline{w'^3} \cong \overline{w'^3}^e + \sigma(1-\sigma)(1-2\sigma)(w_u - w_e)^3, \quad (3)$$

where the subscripts and superscripts $u$ and $e$ refer to the updrafts and the complementary environmental part and $\sigma$ is the fractional area occupied by updrafts. The global area average satisfies $\overline{w} = \sigma w_u + (1-\sigma)w_e = 0$. Without losing much generality it can be written that

$$\overline{w'e} \cong \overline{w'e}^e + \frac{1}{2}\sigma\frac{1-2\sigma}{(1-\sigma)^2}w_u^3. \quad (4)$$

In Eq. (4) the environmental flux (first term on the rhs) accounts mostly for the fluxes of horizontal components of TKE ($\overline{w'u'^2}$ and $\overline{w'v'^2}$) but also includes the environmental part of the $w'$ triple correlation [first rhs term in Eq. (3)]. Based on Eq. (4) and assuming $\sigma$ is constant, a final form of the new EDMF parameterization of turbulent transport of TKE can be formulated:

$$\underbrace{\frac{\partial\overline{w'e}}{\partial z} + \frac{1}{\rho}\frac{\partial\overline{w'p'}}{\partial z}}_{\text{TKE transport}} \cong \underbrace{\frac{\partial}{\partial z}\left(-K\frac{\partial e}{\partial z}\right)}_{\text{ED term}} + \underbrace{\frac{3}{2}\sigma w_u^2\frac{\partial w_u}{\partial z}\left[1 - \frac{\sigma^2}{(1-\sigma)^2}\right]}_{\text{MF term}}, \quad (5)$$

where $K$ is the diffusion coefficient for TKE.

The vertical turbulent transport of TKE is decomposed into an ED and an MF term. The MF term becomes zero when $\sigma$ approaches 0.5. This can be interpreted as a situation when there is no clear distinction between updrafts and the complementary environmental part as in a weak mixing scenario or when turbulence is being mainly generated by horizontal shear. In such cases the updraft environment decomposition loses its foundation. In convectively driven boundary layers, on the other hand, $\sigma$ has been traditionally chosen to be about 0.1. Such a value is often assumed in EDMF parameterizations for scalar fluxes (Soares et al. 2004; Siebesma et al. 2007; Neggers et al. 2009). Small $\sigma$ implies that the expression in the square brackets in the MF term can be approximated as 1. An important advantage of the MF term is that it only depends on the updraft velocity, which can be readily derived from the existing parameterizations. The updraft velocity is already a key component of many EDMF parameterizations, where it is derived using modified versions of Simpson and Wiggert's (1969) equation. These parameterizations are usually sufficiently accurate, as indicated by various comparisons against $w_u$ derived from LES results (e.g., Soares et al. 2004; Siebesma et al. 2007; Neggers et al. 2009).

Figure 2 presents the MF component from Eq. (5), normalized and averaged, as diagnosed from LES results, together with the transport calculated from LES. The updraft fraction is set to 0.13 for the reasons described later in this section. Additionally, the MF term obtained with the updraft fraction 0.1 is also presented. The MF term follows the LES transport remarkably well, having a similar vertical structure and a comparable magnitude to the LES values. The similarities are even more pronounced when compared with the projected ED transport presented in Fig. 1. A more detailed evaluation shows some minor disagreements; in particular, the MF term slightly overestimates TKE removal from the surface layer and underestimates the transport close to the inversion. It also becomes a TKE source term above around 0.4 of the CBL height, a bit lower than LES. When integrated over the whole CBL the MF term vanishes, preserving an important attribute of the actual TKE vertical transport. When an updraft fraction is lowered to a typically used 0.1 value, the results of the MF parameterization remain quite similar, confirming that the MF term produces stable outcomes for the range of $\sigma$ values commonly used by investigators. The resemblance of the MF term to the LES calculated transport suggests its potential application in numerical models as a representation of turbulent transport of TKE. The MF term can be used exclusively or in combination with ED, forming an EDMF framework for TKE modeling.

LES results described in the previous section are used to investigate an optimal updraft fraction for which the total difference between the LES-derived transport and the parameterized MF transport [Eq. (5)] is the smallest. The difference in absolute values is investigated. Figure 3 shows these minimal differences (represented as the fraction of the LES transport) and the corresponding updraft fractions for each LES model output. The crossings of the dashed lines indicate mean values. On average the MF term accounts for 97% of LES transport, with the mean updraft fraction being approximately 0.13. Individual results vary between 80% and 110% and $\sigma$ values range between 0.1 and 0.15. A simple

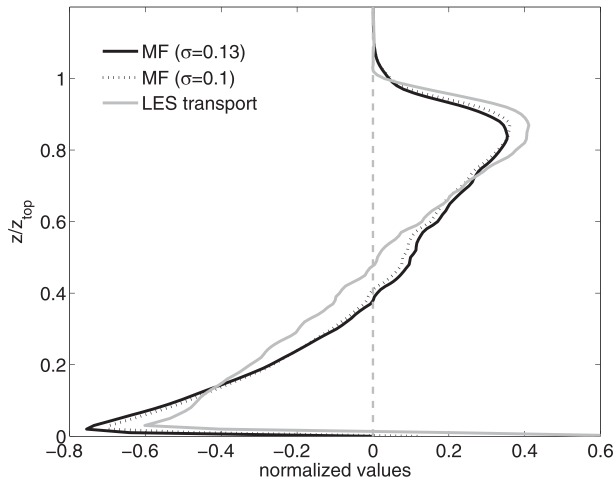


FIG. 2. Normalized and averaged (2–8 h) MF transport of TKE calculated from Eq. (5) with $\sigma = 0.13$ (black line) and $\sigma = 0.1$ (dotted line); the gray line indicates the LES transport term.

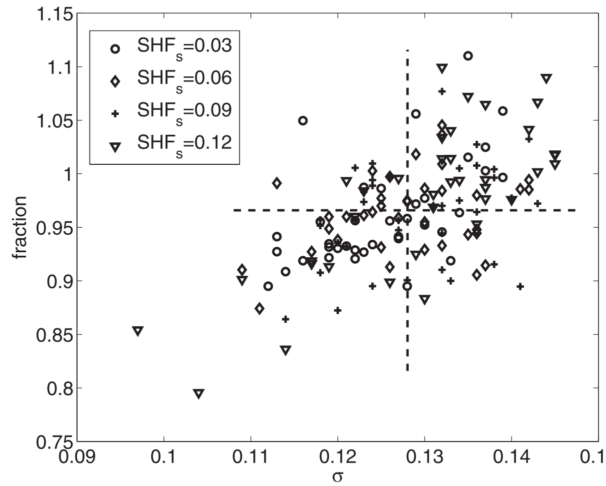


FIG. 3. Maximum fraction of LES transport that can be obtained with the MF parameterization [see Eq. (5)] as a function of the updraft area $\sigma$ for which this maximum transport is achieved. The crossing dashed lines mark the average values.

MF parameterization is therefore able to almost fully resolve the vertical turbulent transport of TKE.

## 4. Parameterization evaluation

The concept of an EDMF transport of TKE introduced in the previous section is evaluated here using a simplified 1D TKE model. The modified TKE prognostic equation has the form

$$\frac{\partial e}{\partial t} = \frac{g}{\overline{\theta}_v}\overline{w'\theta'_v} - \varepsilon - \frac{\partial}{\partial z}\left(-K\frac{\partial e}{\partial z}\right) - \alpha\sigma w_u^2 \frac{\partial w_u}{\partial z}, \quad (6)$$

where $\alpha = 1.5$ is a scaling coefficient and $\sigma = 0.13$. The last two terms represent the ED transport and the MF transport, respectively. An important assumption in the model is that the buoyancy source term is being prescribed using the normalized profile presented in Fig. 1. The updraft vertical velocity, as well as other variables important for the integration, is also prescribed using normalized profiles obtained from LES. These steps allow us to isolate the TKE prognostic equation and concentrate on the performance of the transport terms, without solving prognostic equations for temperature and humidity. The initial state and the boundary conditions are based on the LES results from the simulation with surface heat flux equal to 0.06 K m s$^{-1}$. We use $z_{\text{top}}$ and $w_*$ from the same LES simulation to convert the normalized profiles to actual buoyancy and $\overline{w}_u$ values. The 1D model simulations span between the second and eighth hour of the LES simulation and results after 6-h integration are analyzed. Equation (6) is solved on a regular 10-m grid; the time step is set to 60 s.

Variables that are derived based on model-integrated TKE values include the TKE viscous dissipation and the ED coefficient. The dissipation is parameterized according to

$$\varepsilon = c_\varepsilon \frac{e^{3/2}}{l_\varepsilon}, \quad (7)$$

where $c_\varepsilon$ is a coefficient that can vary in time and $l_\varepsilon = \tau\sqrt{e} = 0.5z_{\text{top}}/w_*\sqrt{e}$ is a dissipation length scale (Teixeira and Cheinet 2004; Witek et al. 2011). Note that no additional scaling is applied to the dissipation length scale, as previously suggested by the LES results presented in Fig. 1. The coefficient $c_\varepsilon$ scales uniformly TKE dissipation and is adjusted at each time step during simulations in a way such that the vertically integrated TKE is equal to that derived from the LES data. Such procedure allows for a more oriented investigation of transport processes, keeping limits on the total turbulence intensity. In practice, the value of $c_\varepsilon$, after initial oscillations related to a fixed choice at the initialization (set to 0.6), remains relatively stable throughout the simulations (results not shown). Those $c_\varepsilon$ values, however, vary slightly among simulations depending on the choice of ED coefficient parameterization.

In this study three different ED coefficient parameterizations found in the literature are used to investigate TKE transport in 1D model simulations. An overview of these formulations is presented in Table 1; a detailed description can be found in the appendix. In general, they were originally formulated as parameterizations of the transfer coefficients of heat, rather than momentum.

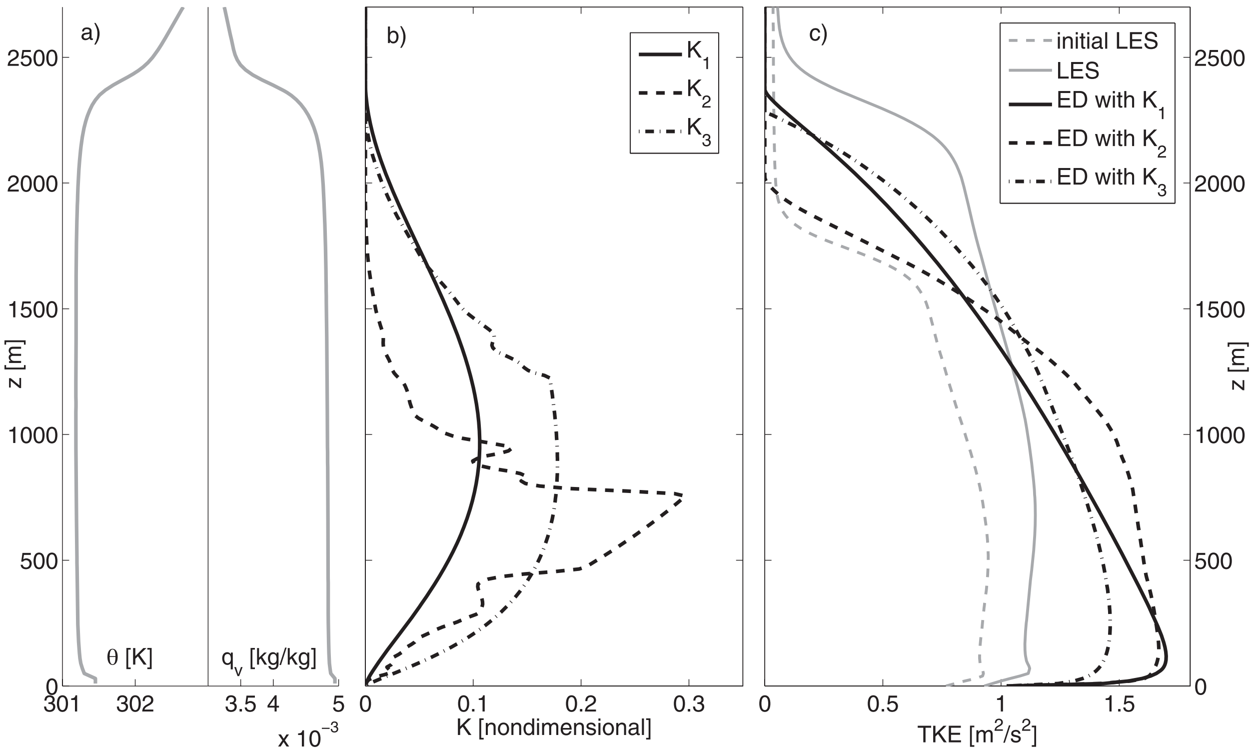


FIG. 4. (a) Potential temperature and humidity profiles at the end of the LES simulation with $SHF_s = 0.06$ K m s$^{-1}$. (b) Different $K$ profiles at the end of 1D model simulations performed with the ED parameterization only. (c) Final TKE profiles as simulated with various ED parameterizations (black lines); initial and final TKE profiles from the reference LES simulation (gray lines).

In our opinion this is an acceptable approach, given the lack of substantial differentiation between them. In short, $K_1$ uses a prescribed profile, whereas $K_2$ and $K_3$ are both based on TKE but employ different mixing length formulations and different surface layer and static stability scaling. The static stability scaling in both cases depends mainly on the Brunt–Väisälä frequency (for definition, see the appendix), which is diagnosed at each time step from the LES-derived temperature and humidity profiles. Stability corrections affect the whole $K_2$ profile, whereas in the case of $K_3$ they only influence the profile in the upper part of the CBL. Examples of the three $K$ parameterizations are presented in Fig. 4b. Strong fluctuations in $K_3$, and some sharper gradients in $K_2$, are consequences of the static stability scaling and computation of the Brunt–Väisälä frequency. Under a close to neutral $\theta$ profile, as depicted in Fig. 4a, the Brunt–Väisälä frequency exhibits very small oscillations around zero. The $S_h$ function proves to be sensitive to these fluctuations, amplifying them and causing substantial variations in the $K_2$ profile. In Bretherton and Park (2009) this feature is not observed, mostly because their temperature profiles are always slightly unstable. They use the ED approach to represent turbulent transport of heat, which cannot accurately simulate neutral or slightly stable stratification in a convective boundary layer. Also, $K_2$ drops substantially above around 800 m and remains small up to the inversion. Again, this is related to a slightly stable $\theta$ stratification simulated by LES that causes the scaling function $S_h$ to be very small.

In Fig. 4c the TKE profiles (black lines) at the eighth hour as simulated with the ED approach only using the three different $K$ parameterizations are presented. The gray lines indicate the initial and the eighth-hour LES results. All 1D model results roughly agree with LES but are clearly not capable of representing the details of the TKE structure. The profiles are too shallow and TKE is highly overestimated in lower parts of the mixed layer. ED transport is not efficient enough to transfer TKE from lower elevations to higher parts of the CBL. For example, the profile obtained with $K_2$ is particularly shallow, which is related to very low $K_2$ values imposed by slightly stable $\theta$ profiles. Adjusting this static stability scaling in $K_2$ could improve its performance to get it closer to the other two $K$ parameterizations. However, our simulations suggest that much closer resemblance with the LES profile cannot be achieved using the ED approach only.

Figure 5a shows results similar to these presented in Fig. 4c, but with the MF transport included in the

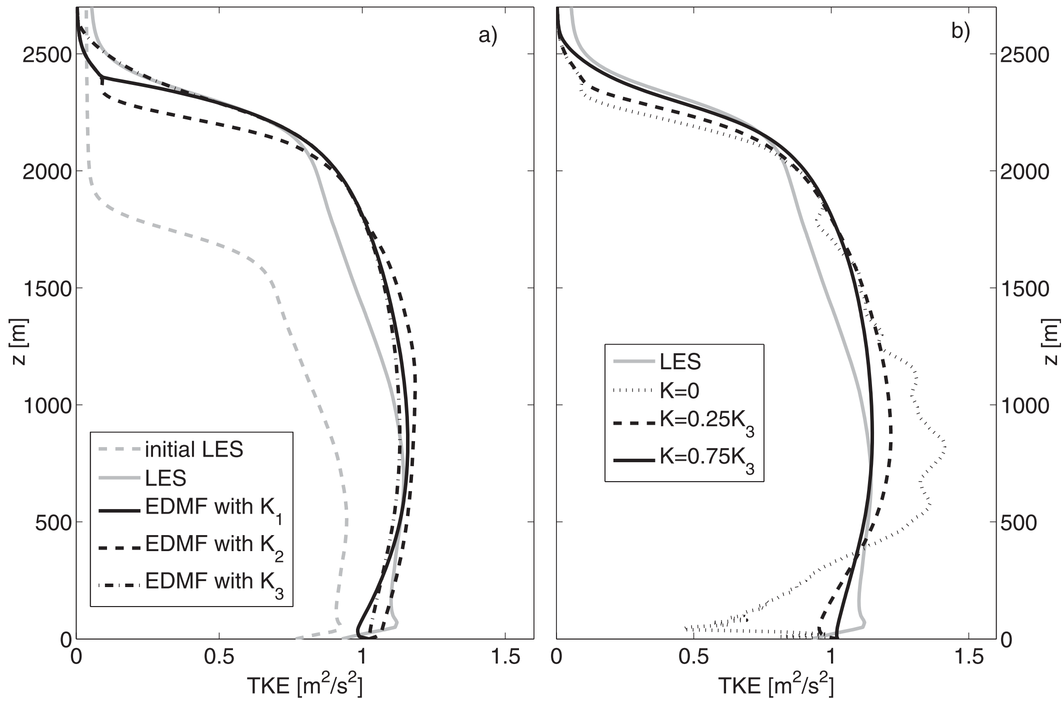


FIG. 5. (a) Final TKE profiles as simulated with various EDMF parameterizations (black lines); initial and final TKE profiles from the reference LES simulation (gray lines). (b) As in (a), but with reduced $K$ values.

simulations. Here $\sigma$ is equal to 0.13 and the $\alpha$ coefficient is set to 1.5. A substantial improvement compared to Fig. 4c is observed. All profiles are much deeper, reaching almost the same height as the LES profiles. The strong TKE overestimation in lower parts of the mixed layer is greatly reduced, and the LES and EDMF profiles are much closer to each other. In particular, the EDMF simulations are capable of reproducing relatively constant TKE values within the mixed layer, compared to the steadily decreasing profiles generated by the ED-only simulations. The addition of the MF term in the TKE transport parameterization substantially enhances the 1D model performance, giving very close agreement with the LES results.

In Fig. 5b the role of the MF term is further investigated to determine whether it could partially or fully substitute for the ED transport. The dotted line shows results of the simulation with the $K$ coefficient set to zero. The MF transport performs very well by itself, surpassing in accuracy the ED parameterizations (see Fig. 4c). The transport overestimation in the surface layer evident in Fig. 2 leads to somehow reduced values of TKE compared to LES. The fairly noisy profile and wiggles are due to the sensitivity of the $w_u$ gradient computation. The addition of diffusive transport (dashed line in Fig. 5b), with $K$ set to $0.25K_3$, ensures a smooth profile and further improves the agreement with LES. Results are even better when $K$ is increased to $0.75K_3$ (solid line in Fig. 5b), producing almost a perfect fit to the LES profile. These results indicate that the EDMF parameterization for TKE transport is potentially capable of achieving realistic simulations of TKE in mesoscale and global atmospheric models.

## 5. Discussion and conclusions

In this study a new approach to the vertical turbulent transport of TKE in convectively driven boundary layers is proposed. The main idea behind the new parameterization is that organized updrafts or convective plumes play an important role in transferring TKE vertically within the CBL. Convection tends to organize itself into localized buoyant updrafts, which on average accelerate in the lower half of the CBL and slow down, losing their momentum, in the upper half. Visible manifestations of these updrafts are cumulus clouds often forming at the top of a CBL. During their life cycle the strongest updrafts interact with the turbulent field surrounding them. One possible interpretation for this interaction is that the updrafts acceleration is supported by the surrounding smaller-scale turbulence, while when the updrafts are losing speed they deposit their energy to the surrounding flow, making it more turbulent. The LES-derived TKE transport term profile somehow confirms this conception: it has negative values where the updrafts accelerate and positive values where they decelerate.

This interpretation suggests that the strongest updrafts might be doing most of the transport of TKE within the CBL. This is the key motivation for applying the updraft environment decomposition to the vertical velocity triple correlation term in the TKE prognostic equation. The procedure creates an additional mass-flux term that can be used to parameterize the vertical transport of TKE. LES results are used to evaluate the approach. The MF term, which is only a function of the updraft vertical velocity, closely resembles the features of the LES-derived vertical transport of TKE. The MF term is, on average, able to resolve 97% of the LES transport, with the mean updraft fraction equal to 0.13. Individual results based on LES output vary between 80% and 110%. By retaining the ED approach, an EDMF framework, similar to those used for the turbulent fluxes of heat and humidity, is formulated for the simulation of TKE.

The new EDMF parameterization is implemented in a simplified 1D model and its performance is evaluated against LES simulations. Different dry convective boundary layer cases are investigated. Three different ED coefficient formulations are used to highlight differences between the ED-only and EDMF approaches. Results show a substantial improvement when the MF term, together with the ED parameterizations, is employed. Even the MF term alone can produce better results than the ED parameterizations by themselves. The new EDMF parameterization is able to represent accurately the LES results even if the ED coefficient is greatly reduced. These results indicate that the proposed EDMF parameterization has a large potential to increase the accuracy of TKE prediction in mesoscale and global atmospheric models.

Finally, some potential caveats of the proposed parameterization can be identified. In particular, the addition of the nonlocal MF TKE transport term, along with the use of the ED local diffusion, introduces some theoretical issues regarding scale separation of the turbulent transport mechanisms. The ED term represents mixing due to small size eddies, whereas the MF term accounts for turbulent transport carried out by large coherent updrafts. The EDMF concept, therefore, implies a distinct scale separation between turbulent transport mechanisms. A conceptual problem arises if, within one scheme, 1) this scale separating EDMF approach is applied to the TKE transport and 2) the ED coefficient is parameterized based on TKE. Such a setup implies that both small- and large-scale turbulent motions contribute to the local diffusion carried out by the ED term. One potential solution to this conundrum would be to simulate separately large- and small-scale TKE and consequently use only the smaller-scale TKE to parameterize the ED coefficient. Such an approach, however, raises many additional theoretical and technical issues that need to be solved, not to mention added complexity. Given the current lack of support of such splitting, we would rather affiliate with a holistic conception of TKE, encompassing all ranges of scales. On the other hand, one can tacitly assume that because of the energy cascade redistributing TKE from the larger to the smaller scales, the ED term might be still proportional to the ''all-scale'' TKE. This proportionality could be different depending on whether a full EDMF or an ED-only approach is applied. In the case of EDMF transport of TKE such an approach works sufficiently well, as demonstrated in the previous sections. For the transport of scalar quantities such as potential temperature or total water mixing ratio we can anticipate a similar behavior, although we do not investigate turbulent transport of these quantities in this study. Further research on this topic should address this scale separation dilemma in a fully interactive scheme, where the EDMF framework is applied for both TKE and scalar quantities alike.

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## APPENDIX

### A Detailed Description of the Three Different Eddy Diffusivity Parameterizations Used in This Study

Following Holtslag (1998),

$$K_1(z) = z_{\mathrm{top}} w_* k \left[\left(\frac{u_*}{w_*}\right)^3 + 39k\frac{z}{z_{\mathrm{top}}}\right]^{1/3} \frac{z}{z_{\mathrm{top}}}\left(1 - \frac{z}{z_{\mathrm{top}}}\right)^2, \tag{A1}$$

where $k = 0.4$ is the von Kármán constant, $z_{\mathrm{top}}$ is the top of the boundary layer, and $u_*$ and $w_*$ are the friction velocity and the convective velocity scale, respectively.

In the free convection limit $u_*$ is derived according to the formula by Abdella and McFarlane (1996), also described in Witek et al. (2011).

After Bretherton and Park (2009),

$$K_2(z) = l_2 S_h \sqrt{e},$$
$$\left(\frac{1}{l_2}\right)^3 = \left(\frac{1}{kz}\right)^3 + \left(\frac{1}{l_\infty}\right)^3,$$
$$S_h = \frac{\alpha_1}{1+\alpha_2 G_h}, \quad G_h = -\frac{N^2 l_2^2}{2e}, \tag{A2}$$

where $l_\infty = 0.17z_{\rm top}$, $\alpha_1 = 0.6986$, $\alpha_2 = -34.6764$, and $N^2 = (g/\theta_v)(\partial\theta_v/\partial z)$ is the squared moist Brunt–Väisälä frequency; also, $G_h$ is additionally restricted at unstable stratifications by $G_h < 0.0233$.

Finally, following Witek et al. (2011),

$$K_3(z) = l_3\sqrt{e},$$
$$\frac{1}{l_3} = \frac{1}{l_a} + \frac{1}{l_b},$$
$$l_a = \tau\sqrt{e} = 0.5\frac{z_{\rm top}}{w_*}\sqrt{e}, \quad l_b = kz\left(1 - 100\frac{z}{L}\right)^{0.2}, \tag{A3}$$

where $L$ is the Monin–Obukhov length defined as $L = -u_*^3\theta_v/(kg\overline{w'\theta_v'}^s)$, $g$ is the acceleration of gravity, and $\overline{w'\theta_v'}^s$ is the buoyancy flux at the surface. We derive $L$ simultaneously with $u_*$ following the procedure by Abdella and McFarlane (1996). Also, $l_a$ is the mixing length introduced by Teixeira and Cheinet (2004), and $l_b$ follows the formulation by Nakanishi (2001). Additionally, $l_3$ is restricted at stable stratifications using the condition by Galperin et al. (1988):

$$l_3 = \min\left(l_3, \frac{0.53\sqrt{e}}{N}\right). \tag{A4}$$

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