A Scale-Adaptive Turbulence Model for the Dry Convective Boundary Layer

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ABSTRACT: A scale-adaptive model is developed for the representation of dry convective boundary layer (CBL) turbulence in numerical models operating at $O(100)$ m to $O(1)$ km horizontal resolution, also known as the model gray zone of the CBL. The new model is constructed based on a planetary boundary layer (PBL) scheme and a large-eddy simulation (LES) closure that are both turbulence kinetic energy-based parameterizations. Scale adaptivity is achieved by “blending” the PBL scheme with the LES closure through an inverse averaging procedure that naturally accounts for vertical variations of the dominant turbulent length scales, hence the gray zone range. High-resolution wide-domain LES benchmark cases covering a broad range of CBL bulk stability are filtered to gray zone resolutions, and analyzed to determine the averaging coefficients. Stability dependence of the dominant length scales is revealed by the analysis and accounted for in the new model. The turbulence model is implemented into a community atmospheric model, and tested for idealized cases. Compared to two established gray zone models, the new model performs equally well under strongly convective conditions, and is more advantageous for the weakly unstable and near neutral CBL.

KEYWORDS: Turbulence; Boundary layer; Large eddy simulations; Subgrid-scale processes

1. Introduction

The model “gray zone” refers to the range of numerical model resolutions that are comparable to the dominant length scale of the flow (Wyngaard 2004, hereafter W04). In the daytime atmospheric boundary layer (ABL), organized convective motion in the form of cells or rolls, depending on the relative strength of heating and vertical wind shear, constitute the dominant boundary layer circulation. The horizontal size of cells or spacing between rolls ($\lambda$) is on the order of the boundary layer depth ($z_i$), usually 1–2 km over land (Kaimal and Finnigan 1994). Therefore, the model gray zone of the convective boundary layer (CBL) is generally defined by horizontal resolution $\Delta \sim \lambda \sim O(z_i)$.

However, observations of energy spectra and cospectra have long before revealed that $z_i$ is not the only dominant length scale of CBL turbulence (Kaimal and Finnigan 1994, chapter 2). Take the turbulent velocity variance as an example. The spectral peak, indicative of the most energetic length scale, of $\sigma_u^2$ scales with height above the ground ($z$) in the surface layer, approaches $O(z_i)$ in the mixed layer, and is limited by the buoyancy length scale $l_b$ in the entrainment zone. The dominant length scale of $\sigma_u^2$ on the other hand, peaks toward the surface and the top of the CBL (see Fig. 7 of Zhou et al. 2017). These findings suggest that the CBL gray zone range must also be height dependent and variable specific. A similar point was also noted in Honnert et al. (2011).

The gray zone presents a challenge to numerical modeling due to the partially resolved and partially subgrid-scale (SGS) nature of turbulence (Honnert et al. 2020). In a mesoscale or global circulation model (GCM) with horizontal spacing $\Delta \sim O(10–100)$ km $\gg \lambda$, a single grid box contains a large number of CBL circulations to warrant a statistical approach to model the ensemble effects of turbulence. The ensemble- or Reynolds-averaged turbulent fluxes are parameterized by planetary boundary layer (PBL) schemes for the Reynolds-averaged Navier–Stokes (RANS) equations adopted by mesoscale models and GCMs. At the other end of the resolution spectrum where $\Delta \ll \lambda$, the most energetic CBL eddies are explicitly resolved. At such fine resolutions, the large-eddy simulation (LES) framework should be adopted (Chow et al. 2019). The effect of SGS turbulence on the resolved flow is modeled with a turbulence closure. In the gray zone where $\Delta$ is comparable to $\lambda$, a grid box contains too few CBL circulations to allow for Reynolds averaging, while such borderline resolution is also too coarse to warrant an LES approach. W04 coined the term “terra incognita” to describe the gray zone that forbids conventional SGS turbulence modeling.

Many numerical weather prediction (NWP) centers are now operating forecast models at convection-permitting horizontal resolutions (usually 4 km or finer) where traditional PBL schemes are barely managing (Ching et al. 2014; Zhou et al. 2014). Further refinement toward kilometer- and subkilometer-scale resolutions subjects NWP models to the CBL gray zone. Continued use of PBL schemes on gray zone grids leads to issues such as overly suppressed resolved turbulence, delayed onset of convection, and misrepresented convective structures (Zhou et al. 2014). Suitable SGS schemes are therefore needed for the representation of gray zone turbulence.

Before introducing gray zone models, it is worth recalling the mathematical foundation that enables gray zone modeling between RANS and LES. As noted above, GCMs and mesoscale models apply Reynolds averaging to arrive at the RANS equations, whereas LES is based on the spatially filtered
Navier–Stokes equations. The RANS and LES equations differ due to the respective averaging operators adopted, and turbulent fluxes defined in each approach. Take the SGS heat flux $\tau_0$ defined in the LES equation, and $T_0$ in the RANS equation, for example,

$$
\tau_0 = \overline{u_i' \theta'} - \overline{u_i \theta'} \quad \text{LES}
$$

$$
T_0 = \overline{u_i' \theta'} \quad \text{PBL}
$$

where $u_i$ are the velocity components, and $\theta$ is the potential temperature. The bar represents a spatial filter, and the hat represents the Reynolds average operator, with primes denoting perturbations from the Reynolds average. Such differences raise fundamental questions regarding the appropriate governing equations and the corresponding definitions of turbulent fluxes for the gray zone.

Germano (1992) first showed that the spatially filtered LES equations are mathematically identical to the statistically averaged RANS equations, provided that the filter commutes with space and time derivatives. For example, one could replace $\overline{u_i \theta'}$ and $\overline{u_i' \theta'}$ in the LES potential temperature equation with $\overline{u_i \theta}$, $\theta$, and $\overline{u_i' \theta}$ to arrive at the corresponding RANS equation, and vice versa. Germano refers to this property as the \textit{averaging invariance of the turbulent equations. It means that the same governing equations in terms of mathematical form but with different filter definitions apply to both RANS and LES.}

W04 further showed that the spatially filtered equations are the appropriate equations for the gray zone, where the filter is restricted to the horizontal plane where SGS homogeneity of turbulence is achieved at mesoscale resolutions. As such, spatially filtered equations converge to RANS equations as the spatial filter converges to the Reynolds average in the limit of $\Delta \to \infty$, so that

$$
\overline{u_i \theta'} - \overline{u_i \theta} = \overline{u_i' \theta'} = \overline{u_i' \theta}.
$$

Based on Leonard’s (1975) decomposition, it is straightforward to show that the Leonard components and cross components of the left-hand side (lhs) are identically zero, leaving only the Reynolds term, hence the equivalence between $\tau_0$ and $T_0$. The work of Germano and Wyngaard together suggests that, with a properly defined spatial filter, the spatially filtered equations apply over the entire resolution spectrum from LES to RANS. This not only simplifies gray zone modeling, but also enables the possibility of adaptive turbulence models across scales (Perot and Gadebusch 2007).

As the name suggests, a scale adaptive turbulence model must be able to correctly modulate its output (i.e., the parameterized turbulent fluxes) based on the grid spacing. Specifically, as turbulence becomes partially resolved at gray zone resolutions, the ensemble-averaged SGS fluxes must decrease with decreasing $\Delta$, while the resolved fluxes increase accordingly (Honnert et al. 2011; Shin and Hong 2013). So far, scale adaptivity is almost always achieved through modifications of existing PBL schemes and/or LES closures. Based on the partitioning between SGS and resolved fluxes, scale-adaptive modifications of PBL schemes usually include an empirical partition function to down-weight the PBL scheme-parameterized fluxes when progressing toward finer resolutions (Boutle et al. 2014; Shin and Hong 2015, hereafter SH15; Ito et al. 2015; Kitamura 2016). LES closures, on the other hand, are based on the definition of a spatial filter that is usually tied to $\Delta$. The scale dependence has been exploited to construct LES closure-based gray zone models (Moeng et al. 2010; Shi et al. 2018; Efstathiou and Plant 2019; Simon et al. 2019). Since scale adaptivity also implies that the model converges to an LES closure at fine spacing, and to a PBL scheme at coarse spacing, more sophisticated models are often constructed by blending a PBL scheme with an LES closure (Boutle et al. 2014; Kurowski and Teixeira 2018, hereafter KT18; Zhang et al. 2018).

Another key requirement of a gray zone model is the ability to represent three-dimensional (3D) turbulence. Traditional PBL schemes assume horizontal homogeneity of SGS turbulence and parameterize only the vertical fluxes (Chow et al. 2019). However, at gray zone resolutions, mixing by horizontal fluxes becomes comparable to that by vertical fluxes, and can no longer be ignored (W04). In this regard, gray zone models based on either LES closure or blending of LES closure and PBL scheme contain parameterized horizontal fluxes from the LES closure, and are more advantageous than gray zone models based on PBL schemes.

Other key ingredients to a successful gray zone model are related to the specific characteristics of gray zone–scale turbulence. These include bulk stability dependence of the dominant turbulent length scales, hence the gray zone range (SH15), anisotropy of turbulent mixing (Kitamura 2015), countergradient fluxes and energy backscatter from SGS to resolved scales (Shi et al. 2019), and stochastic perturbations to represent physical variability at the grid scale (Kober and Craig 2016; Hirt et al. 2019).

In this study, a 3D scale-adaptive turbulence model for the dry CBL is formulated by blending a PBL scheme and an LES closure (section 2). Distinguishing features of the new model include an inverse averaging procedure to achieve scale adaptivity, with the averaging coefficients determined based on an \textit{a priori} analysis of LES benchmark cases (section 3). Stability dependence of the gray zone fluxes is also characterized based on coarse-grained LES data, and is accounted for in the model. Aspects of the gray zone model that require future improvements are documented in section 4. The new model is implemented into a nonhydrostatic community atmospheric model, and its performance is evaluated in section 5, followed by a brief summary in section 6.

2. Model formulation

This section first introduces an LES closure and a PBL scheme, both of which are TKE-based higher-order parameterizations of turbulence. A gray zone model is formulated by
blending the LES closure with the PBL scheme to achieve scale adaptivity. Distinguishing features of the proposed model is given toward the end. Nomenclature-wise, since many variables and coefficients share the same names but are defined differently, we use lowercase, uppercase, and calligraphic letters to differentiate between those defined for the LES closure, the PBL scheme, and the gray zone model, respectively.

a. The LES closure and the PBL scheme

The LES closure of Moeng (1984, hereafter referred to as TKE-1.5) and the PBL scheme of Bougeault and Lacarrere (1989, hereafter referred to as BouLac) form two pillars of the proposed gray zone model. Both are 1.5-order models that solve a prognostic TKE equation and utilize TKE to parameterize SGS turbulent fluxes. The TKE-1.5 closure is a gradient-diffusion model, where SGS fluxes are parameterized as downgradient fluxes based on the definition of turbulent mixing coefficients, also known as eddy viscosity for momentum and eddy diffusivity for heat and other scalars. Taking the vertical SGS heat flux $\overline{w'\theta'} - \overline{w}\overline{\theta}$ (or $\tau_{\theta\theta}$), for example,

$$\tau_{\theta\theta} = -K_H \frac{\partial \overline{\theta}}{\partial z},$$

(1)

where $K_H$ is the eddy diffusivity of heat, denoted by subscript $H$. The generic LES turbulent mixing coefficient $k$ is formulated as

$$k = l\sqrt{e},$$

(2)

where $e = \overline{(u'v')^2}$ is the SGS TKE, and $l$ is the LES mixing length. Note the absence of a model coefficient on the right-hand side (rhs) of Eq. (2), as it is absorbed into the definition of $l$. Doing so gives a consistent formulation of the mixing coefficient among the LES closure, the PBL scheme, and the gray zone model. On near isotropic grids

$$l = c_k (\Delta_x \Delta_y \Delta_z)^{1/3},$$

(3)

where $c_k = 0.1$. For anisotropic grids ($\Delta_x, \Delta_y \gg \Delta_z$), separate horizontal $l_h = c_k \sqrt{\Delta_x \Delta_y}$ and vertical $l_v = c_k \Delta_z$ length scales can be defined. Under stable stratification, $l$ is further limited by the buoyancy length $l_b = \sqrt{g/\rho_f}$, where $N^2 = (g/\rho_f)(\partial \overline{\theta}/\partial z)$ is the buoyancy frequency. Eddy viscosity $k_M$ and eddy diffusivity $K_H$ are linked by a turbulent Prandtl number $Pr_T = k_M/k_H \approx O(1)$.

The BouLac scheme adopts the same gradient-diffusion framework except for the vertical heat flux, where an additional correction term $\gamma$ is included to account for the countergradient transport of heat against the local vertical gradient of potential temperature (Bougeault and Lacarrere 1989). As such, $\gamma$ is defined only within the CBL, and vanishes above the CBL or under stable conditions. In BouLac, the vertical SGS heat flux $w'\theta'$ (or $\tau_{\theta\theta}$) is parameterized as

$$\tau_{\theta\theta} = -K_H \left( \frac{\partial \overline{\theta}}{\partial z} - \gamma \right),$$

(4)

where $K_H$ is the eddy diffusivity of heat for the PBL scheme. For a TKE-based scheme such as BouLac, the generic mixing coefficient $K$ is parameterized as

$$K = L \sqrt{E},$$

(5)

where $E = \overline{(u')^2}/2$ is the Reynolds-averaged TKE, $L$ is the PBL mixing length formulated as a function of the height above ground $z$, the boundary layer depth $z_a$, and often $E$. Under stable conditions, $L$ is often further limited by a Richardson number-based stability function. Since traditional PBL schemes are essentially 1D single-column models, $K$ and $L$ are defined for the vertical direction only. As the TKE-1.5 closure, $K_M$ and $K_H$ are also linked by the turbulent Prandtl number $Pr_T$, where $Pr_T = 1$ is adopted by the BouLac scheme.

In the original BouLac scheme, $L = C_k \min(L_u, L_d)$, where $C_k = 0.4$ and $L_u$ and $L_d$ represent the upward and downward distances that an undiluted air parcel at height $z$ with a mean $E(z)$ can travel under inertial and buoyancy forces,

$$\int_z^{z_e} \frac{g}{\Theta_0} \left[ \partial (z') - \partial (z) \right] dz' = E(z),$$

(6)

$$\int_z^{z-L_u} \frac{g}{\Theta_0} \left[ \partial (z) - \partial (z') \right] dz' = E(z).$$

(7)

The value of $L_d$ is further limited by $z$. Zhou et al. (2020) proposed an improved mixing length for BouLac, where $L_d$ is replaced with Redelsperger et al.’s (2001) length scale $L_s$ to achieve better agreement with Monin–Obukhov (MO) surface similarity theory,

$$L_s = A \Phi_L (z/L_u),$$

(8)

where $A = 0.465$ is a constant, and $\Phi_L$ is an MO stability function [see Zhou et al. (2020) for details]. In Eq. (5) $L_s$ is constructed by combining $L_u$ and $L_s$ through inverse averaging

$$L = C_k \left[ L_u^{-2} + L_s^{-2} \right]^{-1/2},$$

(9)

where $L$ defined by Eq. (9) is the PBL mixing length used in this study. The $\gamma$ term in Eq. (4) adopts Holtslag and Moeng’s (1991) formulation, where

$$\gamma = \frac{w^2 \theta_s}{w^2 \zeta},$$

(10)

for $z \leq z_c$, and 0 above, $w_s = (g/\Theta_0 H_s z_c)^{1/3}$ and $\theta_s = H_s \theta_a$ are the convective velocity and temperature scales, respectively. The variance profile $w^2 \zeta(z)$ is based on the classic empirical fittings of Lenschow et al. (1980). Note that different formulations of $\gamma$ have been proposed in the literature and there is no consensus on the optimal form. The specific choice of Eq. (10) does affect both the amount and, to a lesser extent, the shape of the countergradient correction flux (Zhou et al. 2018), and subsequently the gray zone model.

Besides the mixing length, TKE-based one-equation schemes also require an additional dissipation length to parameterize the viscous dissipation rate $\varepsilon$, where

$$\varepsilon = \begin{cases} \frac{E^{3/4}}{L_s}, & \text{LES} \\ \frac{E^{3/4}}{L_e}, & \text{PBL}, \end{cases}$$

(11)
where \( l_e \) and \( L_e \) are the dissipation lengths with model coefficients absorbed into their definitions. For the TKE-1.5 closure, 
\[ l_e = l_c e^-x, \]
where \( c_x = 0.093 \). In the BouLac scheme, 
\[ L_e = \sqrt{L_t L_d / C_t}, \]
where \( C_t = 0.71 \).

### b. The new gray zone model

The new gray zone model adopts the gradient-diffusion assumption, consistent with the underlying LES closure and PBL scheme. With the spatially filtered equations for the gray zone (W04), the SGS vertical heat flux \( w_\tau \) (or \( \tau_{g3} \)) is parameterized as

\[
\tau_{g3} = -\mathcal{E} \left( \frac{\partial \theta}{\partial z} - \overline{\gamma} \right). \tag{12}
\]

The countergradient correction term \( \gamma \) in Eq. (4) from the PBL scheme is retained, since nonlocal flux still plays a significant role in the vertical mixing of heat at gray zone resolutions (Shin and Hong 2013; Zhou et al. 2018). The turbulent mixing coefficient \( \mathcal{E} \) is defined by the same generic formulation as the LES closure and the PBL scheme

\[
\mathcal{E} = \mathcal{E} \sqrt{\varepsilon}, \tag{13}
\]

where \( \mathcal{E} \) is the mixing length to be formulated. The value of \( \mathcal{E} \) should converge to the LES length scale \( \ell \) and the PBL mixing length \( L \) as the horizontal grid spacing approaches 0 and \( \infty \), respectively.

Following KT18, an inverse averaging approach is adopted to construct a scale-adaptive mixing length \( \mathcal{E} \) based on its LES and PBL counterparts

\[
\mathcal{E} = [\Gamma^{-\alpha} + (L^2)^{-\alpha}]^{-1/\alpha}, \tag{14}
\]

where \( \alpha > 0 \) is the averaging coefficient, and \( L^2 \) denotes the PBL mixing length \( L \) computed on a horizontal grid of \( \Delta \) spacing. Distinction between \( L^2 \) and \( L \) is necessary for TKE-based PBL schemes, because \( L \) can be grid dependent through inclusion of the grid-dependent SGS TKE in its formulation, which is the case for the BouLac scheme [see Eqs. (6) and (7)]. With inverse averaging, \( \mathcal{E} \) depends more on the smaller of \( L \) and \( L^2 \), so that it smoothly converges to \( L \) at fine LES resolutions and to \( L \) at coarse mesoscale resolutions.

A simplifying assumption is made for Eq. (14) to equate the model constants \( c_k \) and \( C_k \) in the definitions of \( l \) in Eq. (3) and \( L \) in Eq. (9). Note that the original value \( C_k = 0.4 \) is 4 times larger than that of \( c_k = 0.1 \). In the literature, different constant values within the general range between 0.1 and 0.5 have been used for TKE-based LES closure and PBL schemes alike (see Table 1 of KT18). For the proposed model, \( c_k \) and \( C_k \) are both set to 0.35 based on a posteriori evaluations to achieve best agreement with LES benchmark profiles. The same assumption that \( c_k = C_k \) is also made by KT18 for their gray zone model.

The dissipation rate \( \varepsilon \) is parameterized as the inverse average of \( l_e \) and \( L_e \)

\[
\mathcal{E} = \left[ (l_e^{-\alpha} + (L_e^2)^{-\alpha})^{-1/\alpha} \right]. \tag{16}
\]

Similarly, \( \mathcal{E} \) is parameterized as the inverse average of \( l_e \) and \( L_e \)

\[
\mathcal{E} = [l_e^{-\alpha} + (L_e^2)^{-\alpha}]^{-1/\alpha}, \tag{16}
\]

with an averaging coefficient \( \alpha \) to be determined. As for the use of \( L_e^2 \) in Eq. (14), the superscripted \( L_e^2 \) is adopted due to the potential grid dependence of \( L_e \) in TKE-based PBL schemes.

### c. Distinguishing features of the new model

As described in section 1, the more popular approach to construct gray zone models is through the use of flux partition functions (Boutle et al. 2014; SH15; Ito et al. 2015; Kitamura 2016; Zhang et al. 2018). The differences between inverse averaging and flux partition approaches to achieve scale adaptivity is first discussed. In the flux partition approach, \( P_r \) is defined as the SGS portion of the grid-independent Reynolds-averaged total flux \( \tau \), that is the sum of the resolved (\( \tau \)) and SGS (\( \tau \)) fluxes, both of which are grid dependent,

\[
P_r(\Delta z_i) = \frac{\tau(\Delta z_i)}{\rho}'(\Delta z_i) + \frac{\tau(\Delta z_i)}{\rho}'(\Delta z_i) = \frac{\tau(\Delta z_i)}{\rho}'(\Delta z_i) = \frac{\tau(\Delta z_i)}{\rho}'(\Delta z_i). \tag{17}
\]

\( P_r \) is almost always expressed as a similarity function of \( \Delta z_i \) and assumed to be universal for the CBL. It is diagnosed from coarse-grained LES data, and then empirically fitted with an analytical expression. The gray zone SGS flux is then obtained as

\[
\tau(\Delta z_i) = P_r(\Delta z_i) \tau_{PBL}, \tag{18}
\]

where \( \tau_{PBL} \) is the parameterized \( \tau \) produced by a PBL scheme (SH15; Ito et al. 2015). Blended schemes such as Boutle et al. (2014) and Zhang et al. (2018) add a weighted portion of the LES flux to the rhs of Eq. (18) to ensure convergence of \( \tau \) toward \( \tau_{PBL} \) at fine grid spacings,

\[
\tau(\Delta z_i) = P_r(\Delta z_i) \tau_{PBL} + [1 - P_r(\Delta z_i)] \tau_{LES}(\Delta z_i), \tag{19}
\]

although strictly speaking, Eq. (19) is no longer valid given the definition of \( P_r \) by Eq. (17).

The choice of inverse averaging over flux partition for the proposed scheme is primarily based on its suitability with TKE-based higher-order schemes. The flux partition approach as outlined by Eqs. (17) and (18) is suitable for first-order schemes. This is because \( \tau_{PBL} \) in Eq. (18) is supposed to represent the grid-independent total flux \( \tau \) in Eq. (17). This is true for first-order schemes such the YSU scheme used in SH15. However, for higher-order schemes, \( \tau_{PBL} \) is already grid dependent through the inclusion of higher-order turbulent moments in its formulation. For example, \( \tau_{PBL} \) by the BouLac scheme [Eq. (4)] is grid dependent due to the inclusion of \( \sqrt{\varepsilon} \) in the definition of \( K \) [Eq. (5)]. As shown later in section 4, although not as rapidly as \( \tau \), \( \varepsilon \) computed by the BouLac scheme does decrease as the grid spacing is refined, so that the magnitudes of the parameterized \( K \), hence \( \tau_{PBL} \) become smaller than their counterparts computed under single-column mode. As a result, \( \tau(\Delta z_i) \) obtained with \( P_r(\Delta z_i) \) through Eq. (18) is also underestimated. In comparison, inverse averaging is more
advantageous since it is applied to the turbulent mixing length rather than the SGS flux. The grid dependence of the TKE-based PBL scheme can be accounted for when determining the averaging coefficients \( \alpha \) and \( \alpha_e \) as shown later in section 3b.

Second, as discussed in section 1, the dominant turbulent length scale \( \lambda \) that determines the gray zone \( \Delta \) is height dependent in the CBL. This means that the diagnosed \( P_r \) in Eq. (17) is a function of \( \Delta/z \) in the surface layer, \( \Delta/\zeta \), in the mixed layer, and \( \Delta/\ell_b \) in the entrainment zone. In Honnert et al. (2011), analytical expressions of \( P_r(\Delta/\zeta) \) are separately fitted for the three layers of the CBL. In practice, however, flux partition-based gray zone models unanimously ignore height variations and adopt usually a mixed-layer depth-averaged \( P_r(\Delta/\zeta) \) for the entire CBL, most likely due to the complexity involved in fitting multivariate functions \( P(\Delta/z, \Delta/\zeta, \Delta/\ell_b) \). In comparison, inverse averaging of the mixing length naturally accounts for the height dependency of \( \lambda \). For example, in the surface layer where small-scale eddies prevail, \( L \) from the PBL scheme that scales with \( z \) is smaller than \( l \) from the LES closure that scales with \( \Delta \). Inverse averaging will produce an \( L \) that is constrained by \( L \). This results in the appropriate convergence of \( \tau \) toward \( \tau_{PBL} \) on the gray grid where \( \Delta \gg z \) in the surface layer. In the mixed layer where \( \lambda \approx \zeta \), inverse averaging will prefer \( l \) over \( L \) on a gray zone grid, resulting in \( \tau \) being closer to \( \tau_{LES} \).

Since inverse averaging is originally proposed by KT18, distinction between their model and ours also deserves some discussion. Besides the obvious difference in the choice of the base state PBL schemes [the Teixeira and Cheinet (2004) scheme vs the BouLac scheme], the main difference lies in how the averaging coefficients \( \alpha \) and \( \alpha_e \) are determined. In KT18, \( \alpha \) is set to 2 to accelerate “the convergence of \( \zeta \) to its asymptotic limits,” i.e., \( \alpha_e = \alpha \) since their dissipation length is set equal to the mixing length. In contrast, we determine \( \alpha \) and \( \alpha_e \) separately based on a priori analysis of filtered LES data as given in the following section. Another difference is that bulk CBL stability dependence of \( \zeta \), as revealed by the a priori analysis, is also considered in our scheme.

### 3. A priori analysis

In this section, benchmark LES cases and their numerical setup are first introduced. We then outline the procedures to determine the averaging coefficients in the new model. A priori analysis of the coarse-grained LES data is then conducted to complete the new model.

#### a. Benchmark LES cases

A set of high-resolution wide-domain LES cases provides the benchmark data for the proposed model. It includes five CBL and one neutral boundary layer (NBL) cases from the previous study of Zhou et al. (2020), and two additional CBL cases (S10-2 and S10-3) to investigate stability dependence of the SGS fluxes. All simulations model barotropic ABL subjected to constant surface heating. The prescribed surface heat flux \( H_s \) and geostrophic winds \( U_g \) are listed in Table 1. All eight cases together cover a broad stability spectrum measured by the parameter \(-z/L_o\), where \( L_o = -u_t^2 \Theta_0/(\kappa g H_s) \) is the Obukhov length, \( u_t \) is the surface friction velocity, \( \kappa \) and \( g \) are the von Kármán and the gravitational acceleration constants. \(-z/L_o\) is a bulk measure of the relative strength of thermal to mechanical forcings (Lenschow and Stephens 1980), where \( +\infty \) and 0 represent the free convective and the neutral limits, respectively. More cases are intentionally placed in the range of \(-z/L_o \leq 20 \) in order to capture the transition of organized convection between cells and rolls (Salesky et al. 2017).

The initial condition of potential temperature follows Shin and Hong (2013), where an isentropic profile is capped by a sharp inversion between 925 and 1075 m to limit CBL growth. The initial wind profile is geostrophic. The Coriolis parameter is \( 10^{-4} \) s\(^{-1} \), and the surface roughness length is 0.1 m. All CBL cases are conducted over a 10.08 km \( \times \) 10.08 km \( \times \) 2 km domain with 10 m horizontal grid spacing. The vertical spacing is 4 m below 1.3 km and is stretched upward. The NBL case is simulated on a 9.216 km \( \times \) 9.216 km \( \times \) 1.5 km domain with 8 m isotropic grid spacing. All simulations adopt horizontally periodic boundary conditions with Rayleigh damping applied to the top one-quarter of the domain. The 1.5-order TKE closure of Moeng (1984) is used for parameterization of SGS turbulence. Cases starting with B, S, and N in Table 1 reach quasi-steady state after about 2.5, and 8 h, and are run for another 2 h with output saved at every 10 min for analysis. The Advanced Regional Prediction System (ARPS) developed at the Center for Analysis and Prediction of Storms at the University of Oklahoma is used for the simulations (Xue et al. 2000, 2001). ARPS is a nonhydrostatic mesoscale and convective-scale finite-difference NWP model that is also suitable for LES (Chow et al. 2005).

#### b. Determining averaging coefficients in the new model

To determine \( \alpha \) in Eq. (14), we first substitute the mixing coefficients [Eqs. (5) and (13)] into their respective flux parameterizations [Eqs. (4) and (12)], apply Reynolds averaging to Eq. (12), and then divide it by Eq. (4) to arrive at

\[
\frac{\tau_{\alpha_0}}{\tau_{\alpha}} = \frac{\sqrt{\xi(\partial \bar{\theta}/\partial \bar{z} - \gamma)}}{L \sqrt{E(\partial \bar{\theta}/\partial \bar{z} - \gamma)}}
\]

<table>
<thead>
<tr>
<th>Case</th>
<th>( H_s ) (m s(^{-1} ))</th>
<th>( U_g ) (m s(^{-1} ))</th>
<th>(-z/L_o)</th>
</tr>
</thead>
<tbody>
<tr>
<td>B1</td>
<td>0.20</td>
<td>1</td>
<td>( 1.5 \times 10^3 )</td>
</tr>
<tr>
<td>B5</td>
<td>0.20</td>
<td>5</td>
<td>81</td>
</tr>
<tr>
<td>B10</td>
<td>0.20</td>
<td>10</td>
<td>19</td>
</tr>
<tr>
<td>S10-2</td>
<td>0.10</td>
<td>10</td>
<td>9.7</td>
</tr>
<tr>
<td>S10</td>
<td>0.05</td>
<td>10</td>
<td>5.5</td>
</tr>
<tr>
<td>S10-3</td>
<td>0.03</td>
<td>10</td>
<td>3.2</td>
</tr>
<tr>
<td>S15</td>
<td>0.05</td>
<td>15</td>
<td>2.0</td>
</tr>
<tr>
<td>N10</td>
<td>0</td>
<td>10</td>
<td>0</td>
</tr>
</tbody>
</table>
To simplify, the Reynolds average of the product in the numerator on the rhs is approximated by the product of the Reynolds average. Based on a priori analysis, the resulting errors of the approximation is small (results not shown). Next, \( \gamma = \gamma \) is assumed, which means that \( \mathcal{H}_u \gamma \) in Eq. (12) is approximated with \( \mathcal{H}_u \gamma \). The physical interpretation of the approximation is that scale dependence of the countergradient correction flux resides solely in \( \mathcal{H}_u \gamma \) rather than \( \gamma \). It is a reasonable first-order approximation based on Fig. 2a of SH15, where the partition functions of the local and nonlocal vertical heat fluxes are found to be similar. Furthermore, given the grid-independent formulation of \( \mathcal{H}_u \gamma \) in Eq. (10), we ultimately have \( \mathcal{H} = \gamma = \gamma \). In addition, restricting the spatial filter to the horizontal plane following W04, we can replace \( \partial \mathcal{H} / \partial z \) with \( \partial \mathcal{H} / \partial z \) in the numerator. The last terms on the rhs within the parentheses are then cancelled.

After rearrangement, the following expression of the Reynolds-averaged \( \mathcal{D} \) is obtained

\[
\mathcal{D} = \left[ \frac{\mathcal{F}_{d}^2 \left( \sqrt{\mathcal{E}} / \sqrt{\mathcal{E}} \right)}{\mathcal{F}_{d}^2} \right] L/z,
\]

or equivalently

\[
\mathcal{D} = \left( P_{e|e} P_{u|e}^{-1} \right) L / L,
\]

where \( P_{e|e} = \sqrt{\mathcal{F}_{d}^2 / \mathcal{E}} \) is the partition function for \( \sqrt{\mathcal{E}} \) following the definition of \( P \) in Eq. (17). Given the possible grid dependence of \( L \) on the rhs, and to facilitate the application of this equation on an actual gray zone grid where \( L \) is known, both sides are further divided by \( L \) to arrive at the final expression for \( \mathcal{D} \),

\[
\mathcal{D} = \left( P_{e|e} P_{u|e}^{-1} \right) L / L = \mathcal{D} = \left( P_{e|e} P_{u|e}^{-1} \right) L / L,
\]

where \( P_{u|e} \) is defined as \( L^2 / L \) for symbolic consistency. Note that unlike \( P \), \( P_{u|e} \) is dependent on the specific formulation of the PBL mixing length. Equation (20) shows that the overall partition function \( P_{u|e} \) is \( \mathcal{D} / L^2 \) for the mixing length of a TKE-based 1.5-order gray zone model consists of three individual partition functions \( P_{e|e} \), \( P_{u|e} \), and \( P_{u|e} \). The \( -1 \) power on the latter two means that the gray zone mixing length does not need to be down-weighted as much as \( P_{e|e} \) due to the scale awareness of \( \mathcal{E} \), and possibly \( L \) depending on its specific formulation. With the \( P_{u|e} \) diagnosed from the filtered LES data, Eq. (20) is used to determine \( \alpha \) in Eq. (14).

Next, we turn to the dissipation length. As shown by the analysis of Ito et al. (2015), the Reynolds-averaged dissipation rate \( \mathcal{E} \) is independent of the grid spacing across the gray zone (see their Fig. 3a). This is because viscous dissipation occurs at the Kolmogorov scale, which is much smaller compared to the LES grid, let alone the gray zone and mesoscale grids. Therefore,

\[
\mathcal{E} = \left( \frac{\mathcal{F}_{d}^2 \mathcal{E}_{d}^2 \mathcal{E}}{\mathcal{F}_{d}^2} \right) = \mathcal{E} / L.
\]

Approximating Reynolds average of the quotient with the quotient of the Reynolds average following Ito et al. (2015), and then dividing both sides by \( L^2 \) to account for possible grid dependence of \( L \), an expression for \( \mathcal{D} \) is obtained:

\[
\mathcal{D} = \left[ \frac{\mathcal{F}_{d}^2 \left( \sqrt{\mathcal{E}} / \sqrt{\mathcal{E}} \right)}{\mathcal{F}_{d}^2} \right] L / L = \mathcal{D} = \left( P_{e|e} P_{u|e}^{-1} \right) L / L.
\]

Similarly, \( P_{e|e} = \mathcal{D} / L^2 \) is the partition function for the dissipation length, to be diagnosed based on \( P_{e|e} \) and \( P_{u|e} \) from the filtered LES data. Equation (21) can then be used to determine \( \alpha \) in Eq. (16).

c. Analysis of filtered LES data

Based on the procedures outlined above, a priori analysis of the LES data is conducted to determine \( \alpha \) and \( \alpha \). Following Shin and Hong (2013), horizontal box averaging is applied to the reference LES data to obtain the resolved flow field on different horizontal grids. The resolved and SGS fluxes are computed accordingly. Statistics are presented with respect to \( \Delta z_e \), where \( \Delta \) is the horizontal grid spacing, and \( z_e \) is taken as the height of the minimum horizontally averaged total heat flux. Horizontal and time averaging denoted by angle brackets are performed to approximate the Reynolds average following Sullivan and Patton (2011). The approximation is appropriate given the wide LES domain compared to \( z_e \) for quasi-steady state CBLs.

Since \( P_{e|e} \) is determined by \( P_{e|e} \), \( P_{u|e} \), and \( P_{u|e} \), we first present the diagnosed vertical profiles of \( \tau_{e|e} \), \( e \), and \( L^2 \) computed on a representative gray zone grid with \( \Delta z_e = 0.48 \) in Fig. 1. Their counterparts computed by taking the entire domain as a single grid column are also presented for comparison. Four cases are presented in descending order of the bulk stability parameter \( -z_e / \Delta z_e \). The other three cases follow the general trend and are omitted from the plot for clarity. Two-sample Student’s \( t \) tests are performed to examine the statistical significance of the differences between adjacent mean profiles. The differences are found to be significant (to 5% level) between 0.1 \( z_e \) and 0.7 \( z_e \) for all three adjacent pairs. In Figs. 1d and 1e, substantial decreases are seen for both \( \tau_{e|e} \) and \( \mathcal{E} \) on the gray zone grid. The corresponding \( P_{e|e} \) and \( P_{u|e} \) in Figs. 1d and 1e are around 0.5 in the middle of the CBL, suggesting near equal contributions from the resolved and SGS components, justifying the gray zone definition.

We see that \( P_{e|e} \) shows significant variations with height. This is expected because \( z_e \) is the dominant length scale of the mixed layer rather than the entire CBL. In the surface layer where wind shear is strong, energetic eddies responsible for vertical mixing of heat scale with \( z_e \). Therefore, on a grid \( \Delta \sim z_e \gg z_e \), the surface layer is still outside its gray zone even though the mixed layer is already inside. This is reflected in the rapid increase of \( P_{e|e} \) toward unity approaching the surface. A similar
increase is also observed in the entrainment zone where turbulent eddies become limited by stable stratification. Note that the large fluctuations of $P_{tu}$ at 0.8 $z_i$ is due to the diminishing fluxes at these heights as shown in Fig. 1a. The vertical variation of $P_{tu}$ confirms the inadequacy of a single-valued partition function for the entire CBL as discussed in section 2c.

Compared to $P_{tu}$, height variations of $P_e$ in Fig. 1e are much milder. This is a result of the height-dependent partition between the vertical $[\epsilon_v = (1/2)\tau_{\theta_3}]$ and horizontal TKE $[\epsilon_h = (1/2)(\tau_{t11} + \tau_{t22})]$ as explained in the section 1. In the surface layer and the entrainment zone, $\epsilon_v$ is limited by the presence of the surface and the stable stratification, respectively, while $\epsilon_h$ driven by the horizontally divergent organized CBL convection is dominant (Zhou et al. 2019). The size of these horizontal fluctuations scale with $z_i$, and defines the gray zone range to be $O(z_i)$. In the mixed layer, $\epsilon_v$ becomes the major contributor to TKE, and its spectral peak is also of $O(z_i)$. Therefore, unlike $\tau_{\theta_3}$, the gray zone range of $e$ is more consistent throughout the depth of the CBL as can be inferred from Fig. 1e.

Figures 1d and 1e also reveal clear stability dependence of $P_{tu}$ and $P_e$. Both exhibit consistent trends, where $P_s$ increase as $-z/L_s$ decreases. The dependence on $-z/L_s$ is attributed to the different length scales of the organized convective structures from cells ($-1.5z_i$) to rolls ($-3z_i$), leading to stability-related variations with $\Delta/z_i$ (SH15), to be further characterized later (in Fig. 5).

Vertical profiles of the PBL mixing length computed on the gray zone grid $\langle L^3 \rangle$ are presented in Fig. 1c and the partition functions $P_L$ in Fig. 1f. The stability-dependent variations of $\langle L \rangle$, represented by the dashed lines, below 0.4$z_i$ in Fig. 1c is a result of the MO-consistent length scales based on Eq. (8). Such variations also show up in the profiles of $\langle L^3 \rangle$. The fact that $P_L < 1$ in Fig. 1f suggests that $L^3$ does exhibit some grid awareness due to its dependence on $e$ as predicted, although $P_L$ is far less sensitive to $\Delta$ than $P_{tu}$ and $P_e$ are.

The profiles of $P_s$ and $P_L$ together suggests that unlike first-order schemes, higher-order PBL schemes are already scale aware due to direct and indirect inclusion of prognostic higher-order turbulent moments (in this case $e$). This opens up interesting possibilities in the design of higher-order PBL schemes to achieve innate scale adaptivity. For the BouLaC scheme, scale adaptivity acquired through $e$ and $L^3$ (i.e., $P_s/P_L$) is clearly not enough to provide the proper reduction of SGS fluxes (i.e., $P_s$) as $\Delta/z_i$ becomes finer. This is shown in Fig. 2a.
where vertical profiles of the overall partition function \( P_\ell = P_{tu}P_{pe}^{-1}P_m^{-1} \) defined in Eq. (20) are presented. The fact that \( P_\ell < 1 \) suggests the necessity of scale-adaptive modifications to a BouLac-based gray scheme. The same is also true for the partition function of the dissipation length \( P_{tu} = P_{tu0}P_{tu1} \) defined in Eq. (21). In Fig. 2b, \( P_{tu} < 1 \) at all elevations, and its profile resembles that of \( P_{tu0} \), since \( P_{tu} \) is close to unity (not shown). In Fig. 2a, notice that \( P_{\ell} \) exceeds 1 near the surface and the CBL top for all cases. This seemingly unphysical behavior is due to \( P_{\ell} < P_{tu0} \) at these heights. As explained earlier with Fig. 1, it is the different dominant length scales for different turbulent moments that leads to different gray zone resolutions, hence \( P_{tu} \).

Three values of \( \alpha \) and \( \alpha_s \) (1, 2, and 3) are substituted into Eqs. (14) and (16), and the modeled partition functions \( P_{tu0}^{m} \) and \( P_{tu1}^{m} \) are presented in Fig. 2. In general, the a priori–diagnosed profiles fall within the coefficient range between 1 and 3. A value of 2 produces decent agreement with case B1 (representing the free convective CBL) in the mixed layer for both \( P_\ell \) and \( P_{tu} \), while \( \alpha = \alpha_s = 3 \) gives a better fit to the near neutral case S15. In the following, we shall set both \( \alpha \) and \( \alpha_s \) to 2, and make further adjustments to account for stability dependence. Note that \( \alpha \) and \( \alpha_s \) are not limited to integer values. One could obtain \( \alpha \), for example, by minimizing the root-mean-square (rms) difference between \( P_\ell \) and \( P_{tu0}^{m} \). A value of 2 is merely a convenient choice that leads to fairly good approximations.

To assess the extent of grid dependence and to evaluate the choice \( \alpha \) and \( \alpha_s \) made at \( \Delta z_L = 0.48 \) for other resolutions, the mixed-layer-averaged statistics for case B1 as a function of \( \Delta z_L \) is presented in Fig. 3. Other cases give qualitatively similar results and are not presented. In Fig. 3a, all \( P_{tu} \)s that define \( P_\ell \) are plotted. Their relative magnitudes are consistent with the results from \( \Delta z_L = 0.48 \) presented in Figs. 1 and 2. The empirical partition function \( P_{tu0}^{sh15} \) used by SH15 fits \( P_{tu0} \)s rather well, and is appropriate for first-order gray zone models. However, it is clear too restrictive for a TKE-based model, as it does not account for the grid dependence through \( P_{tu} \) nor \( P_L \).

In Fig. 3b, \( P_{tu0} \) is only slightly larger than \( P_{tu0}^{m} \) due to the relatively weak grid dependence of \( P_{tu0} \). The modeled \( P_{tu0}^{m}(\alpha = 2) \) fits the a priori–determined \( P_{tu} \) quite well until \( \Delta z_L \approx 0.3 \), and mildly underpredicts the benchmark curve at finer spacings. In Fig. 3b, \( P_{tu0} \) is only slightly larger than \( P_{tu0}^{m} \) due to the relatively weak grid dependence of \( P_{tu0} \). The modeled \( P_{tu0}^{m}(\alpha = 2) \) fits \( P_{tu0} \) well over the entire resolution range. It also compares well with Ito et al.’s (2015) empirical expression \( P_{tu0}^{ibp} \). It is encouraging that the modeled partition function obtained through inverse averaging is comparable to that obtained from direct curve fitting.

Next, stability dependence of the CBL gray zone is investigated. We focus on \( P_{tu0} \) and \( P_{tu1} \) due to the importance of vertical mixing in the PBL. \( P_{tu0} \) is the partition function for the streamwise vertical momentum flux \( \tau_{1u} \). The mixed-layer-averaged \( P_{tu0} \) and \( P_{tu1} \) for all cases are presented in Fig. 4. In cases B1 and B5, the magnitudes of \( \tau_{1u} \) are small, and the corresponding \( P_{tu0} \)s exhibit large fluctuations, hence not presented. Overall, variations of \( P_{tu0} \) and \( P_{tu1} \) with respect to \( \Delta z_L \) are quite similar for the CBL cases, with the latter being slightly smaller especially at finer resolutions. In addition, \( P_{tu0} \) and \( P_{tu1} \) exhibit similar stability dependence, where both \( P_{tu0} \)s decrease with \( -z_L/L_0 \) at a given \( \Delta z_L \). Based on these findings, we adopt the same averaging procedure as Eq. (20) (with \( \alpha = 2 \)) to obtain the gray zone mixing length of momentum.
Note that in Fig. 4, an abrupt increase is found in $P_{\eta}$, from cases S15 to N10 as surface heating is turned off. This is expected because as the CBL transitions into a neutral state, organized convection that sets the CBL gray zone weakens and disappears eventually. Moeng and Sullivan (1994) suggested that this transition occurs at $-z/L_o \sim 1.5$, while a more recent study of Jayaraman and Brasseur (2018) proposed a critical $-z/L_o \sim 0.4$. The length scale of the most energetic NBL eddies is much smaller compared to $z_e$, resulting in a significant leftward shift of $P_{\eta}$. The same change should also be expected for $P_{\eta}$. The CBL–NBL transition is not well studied in general and is unfortunately not resolved by the current LES cases.

Based on the results presented in Figs. 2–4, bulk stability dependence of $P$ should be considered. SH15 proposed a dimensionless stability parameter $C_s$ to account for variations of the dominant CBL length scale $\alpha$ with respect to $u_a/w_a$, a stability parameter equivalent to $-z/L_o$ through $\kappa(u_a/w_a)^{-3} = -z/L_o$. $C_s(u_a/w_a) = \lambda(u_a/w_a)/\lambda(0)$ is interpreted as the ratio of the dominant mixed-layer length scale $\lambda$ under bulk stability $u_a/w_a$ to that of the free convective boundary layer where $u_a/w_a = 0$. The $P$s are then formulated with respect to the dimensionless spacing $\Delta(C_s, z_e)$ instead of $\Delta z$. In SH15, $C_s$ is formulated based on the qualitative description of the CBL length scales given by Moeng and Sullivan (1994),

$$C_s = a[\tanh(b|u_a/w_a + c| + d) + e], \quad (22)$$

where $a = 0.5$, $b = -80.0$, $c = -0.5$, $d = 14.0$, and $e = 3.0$ are the constants.2

In this study, $C_s$ is diagnosed from the filtered LES data in order to give a universal $P(\Delta(C_s, z_e))$ curve for different stability cases: first, $P^{FC}$ for the free-convective case B1 is taken as the reference case where $C_s = 1$; the mixed-layer-averaged $P$ of another CBL case is plotted as a function of $\Delta(C_s, z_e)$ over a range of $C_s$ values; the rms difference between the leftward-shifted $P(\Delta(C_s, z_e))$ and the reference $P^{FC}$ is minimized over the normalized resolution range of [0.1, 1.0] to determine the best $C_s$ value for maximum overlap of the two curves.

The diagnosed $C_s$ for $P^*$ and $P_{\eta}$, are presented in Fig. 5 for all CBL cases as a function of $u_a/\sqrt{u_a^2 + w_a^2}$, so that 0 and 1 represent the free convective and neutral limits, respectively. $C_s$ diagnosed for $P_{\eta}$ and $P_{\eta}^{*}$, as well as the parameterized $C_s$ by Eq. (22) are also plotted for comparison. The diagnosed $C_s$ for different partition functions are quite similar, and vary almost linearly with $u_a/w_a$ from 0.06 (case B1) up to about 0.6 (case S15). This is different from SH15’s model, which mimics a top-hat function with step changes of the dominant length scale at the cell to roll transition where $u_a/w_a \sim 0.3$, and the CBL to NBL transition where $u_a/w_a \sim 0.7$. The parameter range for $u_a/w_a > 0.6$ ($0 < -z/L_o < 2.0$) is not resolved by the current LES cases, although the neutral case N10 provides a single
case. The legend presents case names and the corresponding dashed lines for CBL cases, with a dash–dotted line for the NBL omitted from the plot due to large fluctuations.

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tions of the gray zone model that are not fully investigated and could be improved in the future. First, the 3D nature of gray zone turbulence requires that all components of the momen-

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4. Aspects of the gray zone model to be improved

This section documents several potentially important aspects of the gray zone model that are not fully investigated and could be improved in the future. First, the 3D nature of gray zone turbulence requires that all components of the momentum flux tensor and scalar flux vector be modeled. Given the significant flux anisotropy in the gray zone (W04), at least separate horizontal (\( \mathcal{K}_h \)) and vertical (\( \mathcal{K}_v \)) mixing coefficients are required for the representation of the tensor/vector

K. Kitamura (2016) further proposed a separate \( \mathcal{K}_{1h} \) for fluxes that involve both horizontal and vertical fluctuations such as \( \tau_{13} \) and \( \tau_{23} \), along with \( \mathcal{K}_{1h} \) and \( \mathcal{K}_{2h} \) for purely horizontal and vertical fluxes. The main difficulty in a blended parameterization of \( \mathcal{K}_h \) is that \( K_h \) is absent in 1D PBL schemes. One option is to adopt \( K_h \) from the 2D Smagorinsky model as is done in Zhang et al. (2018). However, this could be problematic for the representation of CBL turbulence, because the 2D Smagorinsky model was developed for GCMs to represent horizontal fluxes that are due to the horizontal deformation of the mesoscale flow field rather than PBL turbulence (Smagorinsky 1963, 1993). In the proposed model, we follow KT18 to set \( \mathcal{K}_h = \mathcal{K}_v \) without formal justification. Doing so produces the right convergence behavior at the LES resolution limit where SGS turbulence is isotropic. It is also a reasonable first-order approximation for CBL turbulence in the mesoscale limit (Zhou et al. 2017).

With two mixing coefficients, it is also necessary to assess whether separate partition functions are required for horizontal and vertical fluxes. The a priori analyses of Honnert et al. (2011) and Shin and Hong (2013) showed that mixed-layer-averaged \( P_s \) of different fluxes are similar, although individual curve fits were proposed in the former. Based on similar analysis with our LES data, the spread among \( P_s \) for different fluxes is comparable with that due to stability variations (results not shown). Therefore, if stability effects are accounted for, so should interflux variability. However, the proposed model only adopts a single \( P \) derived for the vertical momentum and heat fluxes for simplicity.

Another important point to note about the partition function is that according to its definition [Eq. (17)], \( P \) is diagnosed based on Reynolds-averaged fluxes. Given the partially resolved nature of the gray zone, grid-scale variations of \( P \) must exist. Accounting for such variations can be challenging, and is not considered in this study. When applying \( P \) to the modeled turbulent fluxes, certain gridscale variability is lost, which could be important for processes such as PBL-induced convective initiation (Kober and Craig 2016; Hirt et al. 2019). One possible remedy is to add stochastic perturbations to the gray zone model (Berner et al. 2017).

Next, as a gradient-diffusion-based scheme, the gray zone model also requires a turbulent Prandtl number \( Pr_T \) to differentiate between mixing coefficients for momentum and heat. For atmospheric flows, \( Pr_T \) is often set to a constant value of either 1 or 0.74 in PBL schemes. Previous studies have also shown that mean profiles of the CBL are not sensitive to the value of \( Pr_T \) within a reasonable range (Noh et al. 2003;
Nielsen-Gammon et al. 2010; Yang et al. 2019; Zhou et al. 2020). In the two base models, BouLac uses $Pr_T = 1$, while TKE-1.5 adopts $Pr_T = 0.33$ for the CBL. The gray zone model adopts the BouLac convention for simplicity.

Last but not the least, in the gray zone model, $g$ in Eq. (12) is assumed to be equal to its mesoscale counterpart $g$ in Eq. (4). To improve the estimation of $g$, one could try analyzing budgets of $\tau_{ad}$ in the gray zone, and estimate $g$ accordingly. The difficulty of this approach would be constructing closure assumptions for third-order moments and second-order pressure covariance in the gray zone. Alternatively, one might follow Shin and Hong (2013) and diagnose, through conditional sampling, profiles of the nonlocal fluxes at gray zone resolutions. This would likely lead to a replacement of $g$ in Eq. (10) with that used in SH15 and Zhang et al. (2018), although such $g$ could fail to produce the slightly stable upper mixed layer known to observations (Hu et al. 2019).

5. Evaluation and discussion

The new gray zone model (hereafter referred to as the NEW model) is implemented into the nonhydrostatic Weather Research and Forecasting (WRF) Model (Skamarock et al. 2008), and tested for idealized CBL cases. Its performance is evaluated against benchmark LES profiles, and cross compared with the gray zone models of SH15 and Zhang et al. (2018) (hereafter referred to as the SH and ZH models). Simulations are also performed with the BouLac scheme and the TKE-1.5 closure as the controls. However, it is found that SGS mixing by the TKE-1.5 closure is insufficient at gray zone resolutions, resulting in steep superadiabatic profiles (see also Simon et al. 2019), hence the TKE-1.5 results are not included. For the SH and BouLac schemes, horizontal fluxes are parameterized by the 2D Smagorinsky model.

Four idealized cases from section 3a with identical initial and boundary conditions are conducted at 1 km and 333 m horizontal grid spacings with $40 \times 40 \times 40$ and $80 \times 80 \times 40$ grid points, respectively. The vertical grid spacing is 50 m. The implicit Euler solver is implemented for vertical turbulent mixing to improve numerical stability. The large time steps are 9 s for the 1 km and 3 s for the 333 m simulations. The four cases span a broad stability range from almost free-convective (B1) to near neutral (S15) conditions. Simulation results are horizontally averaged and compared to the reference LES benchmark (abbreviated as REF).

Vertical profiles of the simulated $\theta$ are presented in Fig. 7. Compared to the reference profiles, the new model performs quite well for all four cases. In fact, $\langle \theta \rangle$ from different schemes are all quite close. This is expected for quasi-steady-state gray zone CBL simulations, because as long as there is sufficient vertical mixing, regardless of whether it is of resolved or subgrid nature, well-mixed $\langle \theta \rangle$ profiles are produced (Zhou et al. 2014). The ZH model is somewhat an exception, as it consistently predicts deeper and warmer CBLs, due to stronger SGS

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4 The BouLac scheme is run with Eq. (10) as the countergradient correction term.

5 According to SH15, horizontal fluxes are parameterized with the TKE-1.5 closure. However, in the default WRF setup, PBL schemes and LES closures are mutually exclusive. Running them simultaneously requires code modifications, and is not attempted.
entrainment of free-tropospheric air (results not shown). Simulated profiles of the horizontal wind speeds $\langle U \rangle$ are also in decent agreement with the LES benchmark (results not shown).

Next, second-order turbulence moments are investigated. Statistics are shown only for the resolved fluxes. Evaluation of SGS fluxes yields the same findings, since the total fluxes remain almost unaffected by the SGS scheme in

![Fig. 7](image_url). Horizontally averaged vertical profiles of potential temperature for four CBL cases at (top) 1 km and (bottom) 333 m horizontal resolutions. Each column represents a different case listed in the upper-left corner of each panel.

![Fig. 8](image_url). As in Fig. 7, but for the resolved vertical heat flux.
these quasi-steady state idealized CBL simulations. Figure 8 presents vertical profiles of the resolved heat flux $\langle w'' \theta'' \rangle$, where double primes denote perturbations from the horizontal mean. At 1 km resolution in the top panel, $\langle w'' \theta'' \rangle$ of the new model agree quite well with the benchmark profiles for cases B1 and B10, as do the other two gray zone models. As CBL stability weakens in cases S10 and S15, the new model increasingly underpredicts $\langle w'' \theta'' \rangle$, but the extent of underprediction is even more severe with the SH and ZH models. $\langle w'' \theta'' \rangle$ from BouLac is either too large at strongly convective conditions or too small at weakly unstable conditions. This is a result of the grid-dependent resolved convection with a conventional PBL scheme as explained in Zhou et al. (2014, see their section 5). At 333 m in the lower panel of Fig. 8, the agreement is improved for all models. Overall, the new model produces the best match to the reference profiles.

Note that $\langle w'' \theta'' \rangle$ alone does not reflect the overall quality of the resolved flow. Vertical profiles of $\langle w'^2 \rangle$, $\langle \theta'^2 \rangle$ and the correlation coefficient $\rho_{w\theta}$ in Figs. 9–11 reveal more details of the characteristics of simulated gray zone turbulence. In Fig. 9, except for case B1, all models not only underestimate $\langle w'^2 \rangle$, but the extent of underestimation increases toward neutral stability on the 1 km grid. Among the gray zone models, ZH performs relatively better. As the grid spacing is refined to 333 m, the underestimation is greatly ameliorated for all models, suggesting the overwhelming benefit of improved resolution. For $\langle \theta'^2 \rangle$ in the top panel of Fig. 10, the NEW and ZH profiles switch from overestimation in the strongly convective B cases to underestimation in the strongly sheared S cases. SH underpredicts $\langle \theta'^2 \rangle$ regardless of the CBL stability. This could be due to the use of the 2D Smagorinsky model for horizontal mixing. It is worth pointing out that at near neutral stability, NEW is the only model capable of sustaining resolved $\theta''$ on the 1 km grid, which explains its ability to predict larger amounts of resolved $\langle w'' \theta'' \rangle$ in Figs. 8c and 8d. The 333 m profiles in the bottom panel of Fig. 10 are again in better agreement with the reference profiles compared to the 1 km results.

Figure 11 presents correlation $\rho_{w\theta}$ between the resolved $w''$ and $\theta''$. The gray zone grid is capable of partially resolving organized convection. These coherent structures are associated with nearly perfect positive correlation in the surface and the mixed layer as shown by reference profiles. All models including BouLac reproduce the reference profiles for all cases at both resolutions, with the exception of S15 in Fig. 11d, where some deviations are found for SH, ZH, and BouLac. This is likely related to these models’ inability to resolve $\theta''$ as shown in Fig. 10d. Overall, Fig. 11 suggests that $\rho_{w\theta}$ is not sensitive to the SGS parameterization, as long as there is sufficient amount of resolved motion.

The vertical momentum flux $\langle u'' w'' \rangle$ is more difficult to predict than $\langle w'' \theta'' \rangle$ as shown in Fig. 12. On the 1 km grid, both ZH and NEW greatly overestimate $\langle u'' w'' \rangle$ for both B10 and S10. The $\langle u'' w'' \rangle$ from the SH model agrees better with the LES benchmark, although the predicted peak elevations are too low for both cases. For S15 in Fig. 12c, NEW produces the best profile, while ZH and SH underestimate $\langle u'' w'' \rangle$. The difference between ZH and NEW as a group, and SH is likely due to the treatment of the nonlocal momentum fluxes. Inclusion of a
strong SGS nonlocal momentum flux in SH is likely responsible for the reduction of $u^0 w^0$. On the 333 m grid, NEW outperforms the other models, with its profiles nearly overlapping the reference profiles.

Profiles of the correlation coefficient $\langle \rho_{uw} \rangle$ in Fig. 13 exposes a fundamental issue that is not revealed by inspecting the $\langle u^0 w^0 \rangle$ profiles. On the 1 km grid, the resolved $u'$ and $w'$ are simply too well correlated by all models for all cases.
Even though $\langle u''w'' \rangle$ is modeled relatively well, for example, by the NEW model for case S15 in Fig. 12c, its $\langle p_{uw} \rangle$ in Fig. 13c suggests that the model is giving the right prediction for the wrong reason. In general, $w''$ should be less correlated with $u''$ than with $\theta''$ (cf. the reference curves in Figs. 13 to those in Fig. 11) due to the presence of organized convective circulations (Lenschow and Sun 2007). The overpredicted $\langle p_{uw} \rangle$ on the 1 km grid suggests a shared weakness among all gray zone models. This issue is ameliorated with increased resolution as shown in the bottom panel of Fig. 13.

An evaluation of the gray zone model for different horizontal resolutions is conducted for case B10. 15 additional simulations are performed with horizontal grid spacings of 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 1.0, 1.2, 1.4, 1.6, 1.8, 2.0, 2.2, and 2.4 km. Experiments are concentrated in the 0.2 to 0.8 resolution range where the steepest gradients of $P_s$ are found in Fig. 4. The time steps follow WRF’s recommendation, where $\Delta t$ (in units of seconds) is set to 6.2 (in units of km). In Fig. 14, $P_{uw}$, computed from these simulations are presented together with the LES-diagnosed profile. Overall, $P_{uw}$ obtained from the simulations compare well with the diagnosed profile, although at resolutions $\Delta z_i > 2$, the simulated $P_{uw}$ approach unity faster than the a priori curve. This points to the deficiency of the proposed model to sustain very small amount of resolved turbulence at borderline resolutions approaching the mesoscale limit.

Finally, to assess the differences between inverse averaging and flux partition approaches as discussed in section 3c, an additional experiment is performed with the NEW model, expect that scale adaptivity is achieved through a scalar partition function instead of inverse averaging. Specifically, $P_x$ in Eq. (20) is replaced by its depth average between 0.2$z_i$ and 0.6$z_i$. The two modeled $P_{uv}'s$ for case B10 at 333 m horizontal resolution are presented in Fig. 15a. In Fig. 15b, $\langle w''\theta'' \rangle$ obtained from the scalar partition function is greater in magnitude than that obtained with inverse averaging, especially in the surface layer. This is because the modeled SGS fluxes in the surface layer is oversuppressed by a depth-averaged partition function as shown in Fig. 15a. In the entrainment zone, the difference between two profiles is small. This because the buoyancy-limited mixing length $L_D$ is already quite small there, so that further decreases in $P_{uv}$ has only a minor effect in $\langle w''\theta'' \rangle$.

Overall, the test cases show that the new model is of comparable performance to the SH and ZH models under strongly convective conditions, while in the weakly unstable and near neutral environment, second-order turbulent profiles produced by the new model are generally better. The test cases also reveal characteristics and issues associated with gray zone models in general. First is the overwhelming benefit of increased resolution in the gray zone. When $\Delta z_i$ is refined from $\sim$1 to $\sim$1/3, simulated turbulence statistics improve for all cases. Second, weakly unstable cases are more challenging to simulate than strongly convective cases. The most outstanding example is with $\langle w''^2 \rangle$ (Figs. 9c.d) that is underpredicted by all models alike. Finally, the partially resolved spatial structure of
turbulence is clearly dependent on the SGS model as revealed by the correlation statistics. The overcorrelation between $u''$ and $w''$ for all gray zone models should be investigated in the future.

6. Summary

In this study, a scale-adaptive turbulence model is developed for the representation of gray zone–scale CBL turbulence on $O(100)$ m to $O(1)$ km numerical grids. The model is formulated based on Moeng’s LES closure and the BouLac PBL scheme, both of which are 1.5-order TKE-based models with consistent gradient-diffusion representation of turbulent fluxes. Scale adaptivity is achieved by blending the mixing and dissipation lengths of the LES closure with those of the PBL scheme through an inverse averaging operator. A suite of LES cases covering a broad range of CBL stability are filtered to gray zone resolutions to enable a priori determination of the averaging coefficients. Stability dependence of SGS fluxes due to changes in the dominant CBL convective structures is also investigated. Its effect is partially incorporated into the gray zone model.

The new model is implemented into WRF, and tested for idealized cases. Comparison with two other established gray zone models show that the new model performs equally well under strongly convective conditions, and is more advantageous for the weakly unstable and near neutral CBL. Preliminary analyses also suggest that all gray models suffer from inadequate resolution of gridscale turbulence, leading to overly coherent structures, and misrepresented momentum fluxes. Real simulations over extended periods as well as sensitivity tests are to be conducted to further evaluate and improve the proposed model.

**FIG. 13.** As in Fig. 7, but for the correlation coefficient between the resolved $w''$ and $u''$.

**FIG. 14.** Horizontally averaged, time-averaged, and mixed-layer-averaged $P_{\tau_\text{u}}(\Delta z_i)$ for case B10. The solid black line represents $P_{\tau_\text{u}}$ diagnosed from the filtered LES data. Cross symbols represent $P_{\tau_\text{u}}$ obtained from actual simulations with the proposed gray zone model between 0.2$z_c$ and 0.6$z_c$. 

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