

Third-Order Transport and Nonlocal Turbulence Closures for Convective Boundary Layers*

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ABSTRACT

The turbulence closure problem for convective boundary layers is considered with the chief aim to advance the understanding and modeling of nonlocal transport due to large-scale semiorganized structures. The key role here is played by third-order moments (fluxes of fluxes). The problem is treated by the example of the vertical turbulent flux of potential temperature. An overview is given of various schemes ranging from comparatively simple countergradient-transport formulations to sophisticated turbulence closures based on budget equations for the second-order moments. As an alternative to conventional "turbulent diffusion parameterization" for the flux of flux of potential temperature, a "turbulent advection plus diffusion parameterization" is developed and diagnostically tested against data from a large eddy simulation. Employing this parameterization, the budget equation for the potential temperature flux provides a nonlocal turbulence closure formulation for the flux in question. The solution to this equation in terms of the Green function is nothing but an integral turbulence closure. In particular cases it reduces to closure schemes proposed earlier, for example, the Deardorff countergradient correction closure, the Wyngaard and Weil transport-asymmetry closure employing the second derivative of transported scalar, and the Berkowicz and Prahm integral closure for passive scalars. Moreover, the proposed Green-function solution provides a mathematically rigorous procedure for the Wyngaard decomposition of turbulence statistics into the bottom-up and top-down components. The Green-function decomposition exhibits nonlinear vertical profiles of the bottom-up and top-down components of the potential temperature flux in sharp contrast to universally adopted linear profiles. For modeling applications, the proposed closure should be equipped with recommendations as to how to specify the temperature and vertical velocity variances and the vertical velocity skewness.

1. Introduction

We consider the turbulence closure problem for convective boundary layers (CBLs). For the sake of defi-

nitens and simplicity we restrict our consideration to a horizontally homogeneous dry atmospheric CBL, so as the buoyancy b is proportional to potential temperature θ ; namely, $b = \beta\theta$, where $\beta = g/T$ is the buoyancy parameter, g is the acceleration due to gravity, and T is a reference value of absolute temperature.

For our analysis an important feature of CBL is the presence of three different types of motion, namely, (i) mean flow that is totally organized and plane parallel in the case in question, (ii) large-scale semiorganized structures that embrace the entire CBL (buoyancy-driven cells in shear-free flows or rolls in sheared flows),

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and (iii) chaotic three-dimensional turbulence generated by local velocity shears and buoyancy forces. In the context of the present discussion, the adjective “large scale” implies that the structure’s spatial scale is comparable to the CBL depth. Then the presence of boundaries is inevitably felt, causing anisotropy of the structures and of their transport properties. It is chiefly due to large-scale structures that the nature of vertical transport of potential temperature (buoyancy), momentum, and passive scalars across the CBL is essentially nonlocal. What this means is that vertical fluxes of the above quantities at a given height, z , cannot be fully determined by mean vertical gradients at the same height. The present paper focuses on vertical flux of potential temperature. The fluxes of momentum and passive scalars can be considered in the same spirit.

We recall that conventional expression of the potential temperature flux $\overline{w'\theta'}$, henceforth referred to as the downgradient approximation, reads

$$\overline{w'\theta'} = -K_H \frac{\partial \Theta}{\partial z}, \quad (1)$$

where w' and θ' are fluctuations of vertical velocity and potential temperature (primes denote fluctuating quantities, and overbars denote ensemble averaging), $\partial\Theta/\partial z$ is vertical gradient of mean potential temperature Θ , and K_H is a coefficient called eddy conductivity. The subscript H stands for the word heat ($\overline{w'\theta'}$ is the heat flux divided by the air density and specific heat at constant pressure). This formulation follows from the analogy between turbulent transport and molecular transport. It is sometimes referred to as “the Boussinesq approximation.” Notice that Boussinesq (1877) considered the velocity profile and introduced the concept of turbulent viscosity. The term Boussinesq approximation as applied to the scalar fluxes is somewhat loose. The downgradient approximation, Eq. (1), usually assumes one-to-one correspondence between turbulent fluxes at a given height and other parameters of the flow at the same height. It also assumes simple proportionality of turbulent flux in question to mean gradient of transported property. Strictly speaking, the above analogy is justified only when the turbulent mixing length is much less than the length scale of heterogeneity of the mean flow. This is often not the case. Nevertheless, Eq. (1) was adopted without discussion in a large number of turbulence closures (henceforth referred to as local downgradient closures). Currently it has become clear that such closures fail when applied to convective flows. This has awakened fresh interest in nonlocal closures.

In the present study, we do not develop a turbulence parameterization that may be immediately used for practical applications. Instead, we focus on understanding the physical nature of nonlocal turbulent transport in CBLs. As a first step, we restrict our consideration to the vertical flux of potential temperature (the fluxes of momentum and passive scalars should be considered

separately). We analyze the role of the third-order moment, the flux of the flux of potential temperature, in the second-order potential temperature flux budget. It is the third-order moment that is largely responsible for the nonlocal nature of turbulent transport. We develop (in section 3) a “turbulent advection plus diffusion parameterization” for the third-order moment in question. As well as all conventional parameterizations, the proposed parameterization applies to the situations where mean and second-order turbulence quantities vary strongly with height. In these situations, it represents an extension of the turbulent diffusion formulation based on the quasi-normal “Gaussian” approximation for the fourth-order moments [the most advanced formulation of this kind for the CBL was developed by Canuto et al. (1994)]. As different from the purely diffusion parameterizations, our parameterization contains an “advective” term that is proportional to the vertical velocity skewness. It is due to this term that our parameterization remains in force in case of “perfect” mixing when all z derivatives of the mean and second-order quantities vanish. Parameterizations based on the quasi-normal approximation lead to the third-order moments that are identically zero in this case. The proposed parameterization for the flux of potential temperature flux is compared (in section 4) with data from a large eddy simulation (LES) of CBLs. Employing the above parameterization for the third-order flux, and a conventional parameterization for the pressure gradient–potential temperature covariance, the potential temperature flux budget equation provides a nonlocal turbulence closure for the flux in question. In particular cases it reduces to closure schemes proposed earlier, for example, the countergradient-correction closure (Deardorff 1972), the transport-asymmetry closure employing the second derivative of transported scalar (Wyngaard and Weil 1991), and integral closure similar to that for passive scalars (Berkowicz and Prahm 1979). The proposed closure is diagnostically tested against LES data. The Green-function technique is used (section 5) to analyze local and nonlocal contributions to the vertical flux of potential temperature and to examine decomposition of this flux into bottom-up and top-down components. The Green-function decomposition results in nonlinear profiles of both components, in contrast to conventional linear profiles.

2. Overview

The fact that the downgradient approximation as applied to geophysical turbulent boundary layers is not always satisfactory was recognized nearly simultaneously by Budyko and Yudin (1946) in Russia and Priestley and Swinbank (1947) in Australia. Budyko and Yudin considered the issue in the context of the global heat budget at the earth’s surface. They came to the conclusion that calculations employing Eq. (1) together with a reasonable parameterization for the eddy con-

ductivity K_H in the atmospheric surface layer lead to unbalanced budget. To improve the heat budget calculations they amended Eq. (1), incorporating a correction term, γ_H , on the rhs,

$$\overline{w'\theta'} = -K_H \left(\frac{\partial\Theta}{\partial z} - \gamma_H \right), \quad (2)$$

and provided heuristic arguments in support of correction. They treated γ_H as an “equilibrium potential temperature gradient” presumably inherent in any type of vertical turbulent transport. Priestley and Swinbank proposed the same formulation and also provided arguments clarifying the incorporation of the “countergradient” γ_H to correct the downgradient approximation.

Convincing experimental evidence and theoretical explanation of failure of the downgradient approximation as applied to convective turbulence was given by Deardorff (1966, 1972). In his laboratory experiments on turbulent penetrative convection developing against the stable stratification aloft, positive values of the flux $\overline{w'\theta'}$ were documented in the upper portion of the convective zone where the mean gradient $\partial\Theta/\partial z$ was positive. This obviously contradicted Eq. (1) and clearly demonstrated that potential temperature in the CBL could be transported counter to the gradient, hence the term “countergradient flux.”

To analyze the countergradient transport theoretically, Deardorff (1972) considered the budget equation for $\overline{w'\theta'}$:

$$\frac{\partial \overline{w'\theta'}}{\partial t} = -\frac{\partial \overline{w'^2\theta'}}{\partial z} - \overline{w'^2} \frac{\partial\Theta}{\partial z} + \beta \overline{\theta'^2} - \overline{\theta' \frac{\partial p'}{\partial z}}. \quad (3)$$

Here, t is time and p is kinematic pressure (i.e., pressure divided by reference value of the air density). The terms on the rhs of Eq. (3) describe (i) turbulent transport of the flux in question, (ii) its production or destruction due to the mean temperature gradient, (iii) its production by the buoyancy forces, and (iv) the pressure gradient–temperature covariance, respectively. Deardorff (1972) neglected the nonstationary term and the turbulent transport term, and parameterized the pressure gradient–temperature covariance term in the spirit of the Rotta (1951) hypothesis, namely,

$$-\overline{\theta' \frac{\partial p'}{\partial z}} = -\frac{\overline{w'\theta'}}{\tau_r}, \quad (4)$$

where τ_r is a pressure relaxation timescale analogous to the Rotta return-to-isotropy timescale. By this means Eq. (2) is derived with the eddy conductivity and the countergradient given by

$$K_H = \tau_r \sigma_w^2, \quad \gamma_H = \beta \sigma_\theta^2 / \sigma_w^2, \quad (5)$$

where σ_w^2 and σ_θ^2 are variances of vertical velocity and potential temperature,

$$\sigma_w^2 \equiv \overline{w'^2}, \quad \sigma_\theta^2 \equiv \overline{\theta'^2}. \quad (6)$$

Notice that the Deardorff countergradient-correction

closure is a local closure as both the eddy conductivity K_H and the countergradient γ_H are expressed in terms of local parameters, τ_r , σ_w , and σ_θ . An essential feature of this closure is that the transport term involving the third-order moment, $\overline{\partial w'^2 \theta' / \partial z}$, in Eq. (3) is neglected. It should be realized that the third moments involving w' are precisely the terms that describe vertical turbulent transport (fluxes of fluxes) in budget equations for second moments. These third moments are believed to be responsible for nonlocal contributions to the second moments involving w' , that is, to vertical fluxes of potential temperature, passive scalars, and momentum.

A practically sound semiempirical countergradient-correction closure for the vertical flux of potential temperature in the CBL, and also for fluxes of passive scalars, was developed by Troen and Mahrt (1986). They proposed an expression of the eddy conductivity K_H consistent with the incorporation of a countergradient, γ_H , in Eq. (2), and employed a version of the Deardorff formulation, assuming γ_H to be independent of height in the CBL interior:

$$\gamma_H \propto w_* \theta_* / w_s h = \overline{w'\theta'_0} / w_s h. \quad (7)$$

Here, h is the CBL depth; w_* and θ_* are the Deardorff velocity and temperature scales,

$$w_* = |\beta \overline{w'\theta'_0} h|^{1/3}, \quad \theta_* = |\overline{w'\theta'_0}| / w_*; \quad (8)$$

$\overline{w'\theta'_0}$ is the potential temperature flux at the surface; and $w_s = (u_*^3 + 0.28w_*^3)^{1/3}$ is a “mixed-layer velocity scale” involving both w_* and the surface friction velocity u_* . A few years earlier Therry and Lacarrere (1983) considered the same problem for the potential temperature flux and employed an expression of γ_H that follows from Eq. (7) with w_* in place of w_s . The same depth-constant scaling estimate of γ_H was, in fact, considered already by Deardorff (1972).

More recently Holtslag and Moeng (1991) extended the Deardorff formulation with due regard to the third-order turbulent transport term $-\overline{\partial w'^2 \theta' / \partial z}$ in Eq. (3), employing results from the Moeng and Wyngaard (1989) large eddy simulation of the CBL. Applying the Deardorff scales, Eq. (8), to switch to dimensionless coordinates, they found that the vertical profile of the above term is similar in shape to the vertical profile of the pressure gradient–temperature covariance term:

$$\frac{h}{w_*^2 \theta_*} \left(-\frac{\partial \overline{w'^2 \theta'}}{\partial z} + \overline{\theta' \frac{\partial p'}{\partial z}} \right) \approx a, \quad (9)$$

where a is a dimensionless coefficient shown to be practically constant throughout the most of the shear-free CBL ($a \approx 2$). To parameterize the pressure gradient–temperature covariance term, Holtslag and Moeng employed a generalized version of Eq. (4), namely,

$$-\overline{\theta' \frac{\partial p'}{\partial z}} = -\frac{\overline{w'\theta'}}{\tau_p} - c_7 \beta \overline{\theta'^2}. \quad (10)$$

Here, the pressure relaxation timescale, denoted as τ_p

to distinguish it from the timescale τ_r in Eq. (4), is usually taken proportional to the turbulence energy-dissipation timescale τ ,

$$\tau_p = \tau/c_6, \quad \tau \equiv \overline{q'^2}/2\varepsilon, \quad (11)$$

where $\overline{q'^2} = \overline{u'^2} + \overline{v'^2} + \overline{w'^2}$ is twice the turbulence kinetic energy (TKE), $\overline{u'^2}$ and $\overline{v'^2}$ are the horizontal velocity variances, ε is the TKE dissipation rate, and c_6 is a dimensionless constant. For this and other dimensionless constants we use the notation commonly accepted nowadays (e.g., Andre 1976; Moeng and Randall 1984; Kurbatskii 1988; Canuto et al. 1994). The second term on the rhs of Eq. (11) reflects the effect of buoyancy on the pressure fluctuations, whereas the first term represents destruction of the flux in question due to turbulent-turbulent interactions. For the constant c_7 Holtslag and Moeng adopted the Moeng and Wyngaard (1986) LES estimate, $c_7 \approx 0.5$. With this estimate the buoyancy terms, grouped together into $(1 - 2c_7)\beta\sigma_\theta^2$, drop out from the flux budget equation, Eq. (3). Then the eddy conductivity and the countergradient are

$$K_H \propto \tau_p \sigma_w^2, \quad \gamma_H \propto w_* \overline{w'\theta'_0}/\sigma_w^2 h. \quad (12)$$

By this means, the potential temperature flux $\overline{w'\theta'}$ is expressed through the CBL bulk parameters h and $\overline{w'\theta'_0}$ and empirical functions $\sigma_w(z)$ and $K_H(z)$.

In the Troen and Mahrt (1986) and the Holtslag and Moeng (1991) countergradient-correction closures the nonlocal transport term $-\partial\overline{w'^2\theta'}/\partial z$ in the flux budget equation, Eq. (3), is either neglected or parameterized through an algebraic combination of the second-order moments. As a result the above differential equation turns into an algebraic equation, which is why the closures in question can hardly be considered as truly nonlocal. At the same time they involve nonlocal features of the vertical transport through the CBL bulk parameters, h and $\overline{w'\theta'_0}$. They can therefore be referred to as pseudo nonlocal closures.

In a sense, Eq. (2) presents contribution from large eddies to the potential temperature flux as a countergradient term, $K_H\gamma_H$. Frech and Mahrt (1995) called attention to the fact that the large eddy flux is not immediately related to the small-scale eddy conductivity K_H , and moreover not necessarily directed counter to the gradient. For practical purposes Frech and Mahrt decomposed the vertical flux of a quantity ψ into small-scale (downgradient) and large-scale (generally nongradient) contributions,

$$\overline{w'\psi'} = -K_\psi \frac{\partial\overline{\psi}}{\partial z} + \overline{w'\psi'_L}, \quad (13)$$

and proposed a power-law parameterization for the latter contribution.

Although the present paper focuses on the potential temperature flux, some ideas concerning nonlocal transport of passive scalars are of general importance and merit consideration here. Thus, for the vertical flux of a passive scalar, φ , Berkowicz and Prahm (1979) and

Fiedler (1984) proposed turbulence closures that imply an integral generalization of the downgradient transport hypothesis,

$$\overline{w'\varphi'} = - \int_0^\infty W_\Phi(z, z') \frac{\partial\overline{\Phi}}{\partial z} dz', \quad (14)$$

where W_Φ is a weight function (a sort of turbulent transport velocity), and $\partial\overline{\Phi}/\partial z$ is the mean gradient of the scalar in question. Stull (1988) developed a similar type of finite-difference closure that involves so-called “transilient matrix” playing the same role as the weight function in Eq. (14). Here, the key problem is how to specify the weight function or transilient matrix.

An important step toward better understanding of the physical nature of nonlocal transport properties of convective flows was made by Wyngaard (1983) and Wyngaard and Brost (1984). They found that vertical diffusion of a dynamically passive scalar through the CBL is a superposition of two processes, namely, a “bottom-up diffusion” due to the buoyancy-driven plumes (updrafts) and a “top-down diffusion” due to the compensating subsidence motions (downdrafts). They also called attention to essential asymmetry in large-scale convective structures. As shown by LES, updrafts are more narrow and energetic than downdrafts, which is why kinetic energy is transported upward almost throughout the entire CBL. Quantitatively, the above asymmetry is characterized by dimensionless third moments called skewness, first of all by the vertical velocity skewness, $S_w = \overline{w'^3}/\overline{w'^2}^{3/2}$.

With these prerequisites, Wyngaard and Weil (1991) developed a Lagrangian formulation for turbulent diffusion, employing S_w to account for the above transport asymmetry of the CBL. They derived an expression of the vertical flux of a passive scalar, φ , similar to Eq. (2) with the eddy diffusivity K_Φ and the nongradient correction γ_Φ given by

$$K_\Phi = \tau_L \sigma_w^2, \quad \gamma_\Phi = S_w \sigma_w \tau_L \frac{\partial^2\overline{\Phi}}{\partial z^2}, \quad (15)$$

where τ_L is a Lagrangian integral timescale. Notice that the term including the second derivative of the mean concentration of scalar in question, $\partial^2\overline{\Phi}/\partial z^2$, can be of any sign. We therefore call this term nongradient rather than countergradient.

It is clear from the above discussion that the key role in the nature of large-scale nonlocal fluxes is played by the fluxes of fluxes represented by third moments, such as $\overline{w'^2\theta'}$. In higher-order closures (e.g., Zeman 1975; Zeman and Lumley 1976; Andre 1976; Moeng and Randall 1984; Kurbatskii 1988; Lykossov 1990; Canuto et al. 1994) the third moments are determined using appropriate budget equations, whereas the fourth moments involved are usually expressed through quasi-normal (Gaussian) approximation [see Eq. (A3) in appendix A]. This approximation was for the first time applied to homogeneous isotropic turbulence by Mil-

lionshchikov (1941), and hence it is often referred to as the Millionshchikov hypothesis.

Canuto et al. (1994) provided the most systematic derivation of this kind for the CBL, employing the above quasi-normal approximation. They derived a new set of diagnostic equations that show a universal structure of the third-order moments. All of them turn out to be linear combinations of the derivatives of all second-order moments, $\overline{w'^2}$, $\overline{w'\theta'}$, $\overline{\theta'^2}$, and $\overline{q'^2}$, multiplied by appropriate turbulent exchange coefficients. In particular, the Canuto et al. equation for $\overline{w'^2\theta'}$ reads

$$-\beta\tau\overline{w'^2\theta'} = \beta\tau A_1 \frac{\partial \overline{w'\theta'}}{\partial z} + A_2 \frac{\partial \overline{w'^2}}{\partial z} + (\beta\tau)^2 A_3 \frac{\partial \overline{\theta'^2}}{\partial z} + A_4 \frac{\partial \overline{q'^2}}{\partial z}, \quad (16)$$

where A_i ($i = 1, 2, 3, 4$) are turbulent exchange coefficients given by

$$A_i = A_{i1}\tau\overline{w'^2} + A_{i2}\beta\tau^2\overline{w'\theta'}, \quad (17)$$

and A_{i1} and A_{i2} are given dimensionless functions of the dimensionless combination $\tau^2\beta\partial\Theta/\partial z$. Similar expressions are derived for other third moments. The exchange coefficients given by Eq. (17) consist of a standard part, $\propto\tau\overline{w'^2}$ [cf. Eqs. (5a) and (12a)], and an additional part, $\propto\beta\tau^2\overline{w'\theta'}$, due to the buoyancy flux. The latter part was already introduced by Zeman and Lumley (1976) and Lumley (1978).

3. Turbulent advection plus diffusion hypothesis for fluxes of fluxes

It is obvious that any parameterization or closure hypotheses, including those based on empirical evidence, should be consistent with requirements of (i) dimension, (ii) tensor invariance, (iii) symmetry, and (iv) realizability. In other words, the rhs of any expression claimed to be physically grounded should have the same dimension, tensor–vector nature, and properties of symmetry as the lhs. Furthermore, empirical dimensionless coefficients in any expression of a statistical moment of turbulence through other moments should satisfy the conditions of realizability. The above comments are especially important considering that turbulence closures are very often developed and verified for simple flows and then extended to more complex flows just with a hope that general features of turbulent transport are caught. Such a hope is unjustified as long as physical requirements are violated.

The most advanced “turbulent diffusion parameterization” for the third moments based on the quasi-normal approximation for the fourth-order moments, proposed by Canuto et al. (1994), evidently satisfies the above physical requirements (i), (ii), and (iii). One could expect that it also satisfies the realizability requirement (iv), although it is not explicitly stated in the paper cited.

As far as the underlying physical concept is concerned, Eqs. (16) and (17) represent a gradient formulation, as the flux of a given second-order quantity depends on the gradients of second-order moments. The Canuto et al. formulation fits LES data very well in the near-boundary zones where pronounced gradients of the second moments are observed, namely, close to the surface and at the inversion base. At the same time the Canuto et al. (1994) Fig. 10 shows that modeled values of $\overline{w'^2\theta'}$ diverge from LES values in the CBL interior. In other words, the third moment $\overline{w'^2\theta'}$ immediately responsible for the nonlocal turbulent transport of potential temperature is best parameterized in the regions of strong gradients, that is, in the regions where it is of minor importance (as the nonlocal contribution to vertical transport of potential temperature is comparatively small). In the CBL interior, however, where gradients are small and nonlocal transport dominates, the turbulent diffusion parameterization of $\overline{w'^2\theta'}$ has not met with success.

As an alternative we propose a turbulent advection plus diffusion parameterization equally applicable to both the near-boundary regions and the CBL interior. To this end, we separately consider two limiting cases. One is the case of perfect mixing where the vertical gradients of the mean and second-order quantities vanish. The opposite case is where these gradients are strong. Below we show that the two different models describing these two cases cannot be reduced to each other.

a. Symmetry arguments for turbulent advection formulation

We first consider the CBL interior, where mean gradients vanish and nonlocal transport dominates. To describe this region, we develop a “turbulent advection parameterization” for the flux of the flux of potential temperature. We assume that beyond the boundary zones, the heat flux is primarily transported by large eddies (rather than diffused by small-scale turbulence) so that $\overline{w'^2\theta'}$ can be expressed as the second-order flux involved, multiplied by a turbulence velocity, w_a , namely,

$$\overline{w'^2\theta'} = C_\theta w_a \overline{w'\theta'}, \quad (18)$$

where C_θ is a dimensionless constant of order 1. The tensor nature of the lhs of Eq. (18) suggests that the rhs must be a component of the second-order tensor. This tensor is formed as a tensor product of the two vector quantities, the temperature flux, and the turbulence velocity. The vertical components of these vectors are $\overline{w'\theta'}$ and w_a , respectively. Then such a seemingly natural candidate for the role of w_a as the scalar rms vertical velocity, σ_w , is inapt. The simplest expression of w_a consistent with the tensor-invariance requirement reads

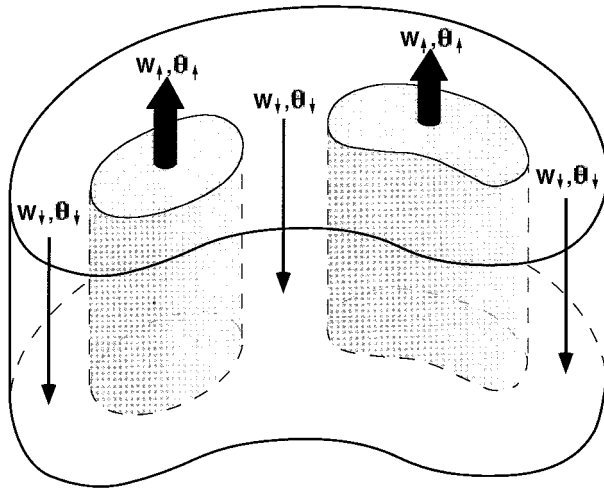


FIG. 1. Schematic illustration of the bimodal bottom-up-top-down turbulence model. For visual demonstration the probabilities P_{\downarrow} and P_{\uparrow} are identified with squares occupied by updrafts and downdrafts.

$$w_a = \overline{w'^3} / \overline{w'^2} \equiv S_w \sigma_w, \quad (19)$$

where S_w is the vertical velocity skewness.¹ We can therefore refer to w_a as to “large-eddy skewed-turbulence advection velocity” (LEST advection velocity).

b. Bimodal bottom-up-top-down model of turbulent advection

Apart from the above phenomenological derivation, the turbulent advection formulation, Eqs. (18) and (19), is derived from a bimodal bottom-up-top-down turbulence model that accounts for the transport asymmetry of the CBL [for other purposes the same model was already employed by Wyngaard (1987)]. As shown in Fig. 1, we adopt (i) that positive and negative vertical velocity fluctuations, w_{\uparrow} and w_{\downarrow} take place with the probabilities P_{\uparrow} and P_{\downarrow} respectively; and (ii) that the potential temperature fluctuations, θ_{\uparrow} and θ_{\downarrow} , are characterized by the same probabilities, P_{\uparrow} and P_{\downarrow} , so that the joint probability density $P_{w\theta}$ is

$$P_{w\theta} = P_{\uparrow} \delta(w' - w_{\uparrow}) \delta(\theta' - \theta_{\uparrow}) + P_{\downarrow} \delta(w' - w_{\downarrow}) \delta(\theta' - \theta_{\downarrow}), \quad (20)$$

where $\delta(x)$ is the Dirac delta function. The model obviously yields the equations

¹ Compare arguments by Wyngaard (1983) and Wyngaard and Brost (1984) in favor of the transport asymmetry of the CBL, and incorporation of S_w in the Wyngaard and Weil (1991) turbulence closure to account for the asymmetry.

$$P_{\uparrow} + P_{\downarrow} = 1, \quad (21)$$

$$w_{\uparrow} P_{\uparrow} + w_{\downarrow} P_{\downarrow} = 0, \quad w_{\uparrow}^2 P_{\uparrow} + w_{\downarrow}^2 P_{\downarrow} = \sigma_w^2, \\ w_{\uparrow}^3 P_{\uparrow} + w_{\downarrow}^3 P_{\downarrow} = S_w \sigma_w^3, \quad (22)$$

$$\theta_{\uparrow} P_{\uparrow} + \theta_{\downarrow} P_{\downarrow} = 0, \quad \theta_{\uparrow}^2 P_{\uparrow} + \theta_{\downarrow}^2 P_{\downarrow} = \sigma_{\theta}^2, \quad (23)$$

which specify the parameters P_{\uparrow} , P_{\downarrow} , w_{\uparrow} , w_{\downarrow} , θ_{\uparrow} , and θ_{\downarrow} . Then, our parameterization for $\overline{w'^2 \theta'}$, Eqs. (18) and (19), written as $\overline{(w'^2)(w'^2 \theta')} = C_{\theta} \overline{(w'^3)} \overline{(w' \theta')}$, is immediately proved for $C_{\theta} = 1$ by substituting the expressions of the rhs and the lhs that follow from Eqs. (21)–(23) and by performing identical transformations.

The above derivation of the turbulence advection formulation for $\overline{w'^2 \theta'}$, Eqs. (18) and (19) with $C_{\theta} = 1$, was given by Zilitinkevich et al. (1997) and independently by Abdella and McFarlane (1997). The latter authors derived the expression of $\overline{w'^2 \theta'}$ [Eq. (19) in Abdella and McFarlane (1997)] employing a “convective mass-flux model,” which differs from our bimodal bottom-up-top-down turbulence model, Eqs. (21)–(23), only in that it employs fractional areas occupied by updrafts and downdrafts [a and $(1 - a)$ in Abdella and McFarlane (1997)] rather than probabilities P_{\uparrow} and P_{\downarrow} (cf. Fig. 1 in which fractional areas are identified with probabilities).

Remember now that in nonskewed turbulence, our turbulent advection model predicts no vertical transport of the potential temperature flux and it should be replaced by one or the other turbulence diffusion formulation. Clearly, a turbulence closure that claims to be realistic and practically sound should embrace both the turbulent advection and the turbulent diffusion formulations.

c. Interpolation between advection and diffusion limits

To guess a reasonable functional form for an advection plus diffusion turbulence closure we consider the opposite limiting case, where vertical gradients of both mean quantities and second-order moments are strong. Then, an expression of the flux of flux, $\overline{w'^2 \theta'}$, is derived from the third-order-moment budget equations employing the quasi-normal approximation for the fourth-order moments (the Millionschikov hypothesis). Keeping $\overline{w'^3}$ in its explicit form, after some algebra and simplification (see appendix B) the resulting expression reads

$$\overline{w'^2 \theta'} = \frac{1}{3} \frac{\overline{w'^3}}{\overline{w'^2}} \overline{w' \theta'} - \frac{1}{2} \tau \overline{w'^3} \frac{\partial \Theta}{\partial z} - K_{w\theta} \frac{\partial \overline{w' \theta'}}{\partial z}, \quad (24)$$

where $K_{w\theta} \propto \tau \overline{w'^2}$ is an appropriate turbulent diffusivity. Remember that Eq. (24) is nothing but a gradient diffusion formulation. The use of the quasi-normal approximation leads to the expression of the triple moment $\overline{w'^3}$ in terms of combination of z derivatives of the second moments involved (see, e.g., Canuto et al. 1994).

In order to derive a formulation suitable throughout the entire convective zone, we interpolate between the advection transport formulation, Eqs. (18) and (19), and the diffusion transport formulation, Eq. (24). The result is

$$\overline{w'^2\theta'} = w_a \left(C_\theta \overline{w'\theta'} - C_k K_{w\theta} \frac{\partial \Theta}{\partial z} \right) - K_{w\theta} \frac{\partial \overline{w'\theta'}}{\partial z}, \quad (25)$$

where C_θ and C_k are dimensionless constants.

The following points concerning Eq. (25) and the way it is arrived at should be discussed in some detail. One might wonder whether there is any advantage to keep the third-order moment $\overline{w'^3}$ in its explicit form on the rhs of Eq. (25).

Consider first the case where mean and second-order quantities vary strongly with height. In such a case, one or the other gradient model should hold. It should be possible to express $\overline{w'^3}$ (and, therefore, also the LEST velocity w_a) in terms of combination of z derivatives of the second moments (see Canuto et al. 1994). Then, Eq. (24) is nothing but a gradient approximation written in a different form. Consider then the opposite case of perfect mixing where all z derivatives of the mean and second-order quantities are zero. In this case, Eqs. (B1)–(B4) (appendix B) based on the quasi-normal approximation lead to the third-order moments that are identically zero. This is not the case for the bimodal bottom-up–top-down model, Eqs. (20)–(23), which remains in force and suggests that $\overline{w'^3}$ should explicitly appear in the parameterization for $\overline{w'^2\theta'}$. Certainly, the problem of parameterization of $\overline{w'^3}$ remains. The authors should admit that they have no definitive answer at the moment. An important observation, however, is that the bimodal bottom-up–top-down turbulence model and the gradient model based on the quasi-normal approximation are suitable for the two “irreconcilable” limiting cases. These models cannot be reduced to each other.

Free convection in the atmospheric PBL represents an intermediate case where turbulence is strongly non-Gaussian but the vertical variations of the second-order quantities remain. In the light of the above discussion, the derivations based on the quasi-normal approximation and the bimodal bottom-up–top-down model should be considered as the leading arguments that suggest the form of the terms to be included into parameterization for the triple moment in question. Equation (25) should then be considered as a reasonable interpolation formula that should obey firm physical constraints and, importantly, should fit empirical and numerical data.

4. Comparison with LES data

In this section we compare the turbulent advection plus diffusion parameterization, Eq. (25), with data from an LES of the CBL. The LES model used in the present study was developed by Moeng (1984) and modified by

Moeng and Wyngaard (1988). Detailed description of the model can be found in the papers cited.

The model solves filtered Navier–Stokes equations using a mixed finite-difference pseudospectral method. Periodic boundary conditions are used in both horizontal directions. At the underlying surface, the potential temperature flux is prescribed and velocities are set to zero. Horizontally averaged flux-profile relationships between the surface and the first grid level above the surface match the Monin–Obukhov similarity theory. The local, fluctuating fluxes of heat and momentum are related to the fluctuating velocity and temperature at the first grid level through a “local similarity rule” (see Moeng 1984, for details). The subgrid-scale parameterization is based on a prognostic equation for the subgrid-scale turbulence kinetic energy. Derivatives in the x and y horizontal directions are evaluated pseudospectrally. The upper $\frac{1}{3}$ of wavenumbers are truncated in Fourier space for dealiasing. Centered finite differences on a uniform vertical grid are used with the vertical velocity and subgrid-scale turbulence energy staggered with respect to other variables (horizontal velocity components, potential temperature, and pressure). The Adams–Bashforth scheme is used for time stepping and the Poisson equation for pressure is solved through a mixed fast Fourier and finite-difference technique.

Two archetypes of the surface-heating-driven convective boundary layer were generated, hereafter referred to as cases “I” and “II.” In case I, the domain size is $5000 \times 5000 \times 2000$ m in the x , y , and z directions, respectively, and 96 grid points are used in each direction. The CBL is capped by a strong temperature inversion above which the temperature increases linearly with height. At the upper boundary of the numerical domain, the subgrid-scale turbulence energy is set to zero, the temperature lapse rate is prescribed, free slip for the horizontal velocity components is used, and the radiation upper boundary conditions are applied, which allow internal gravity waves to leave the system. The initial temperature profile in case I consists of a mixed layer of depth 1000 m and temperature 300 K capped by strong temperature inversion where temperature increases linearly by 8 K over six grid intervals, with the lapse rate 3×10^{-3} K m^{-1} above the inversion.

In case II, the domain size is $4000 \times 4000 \times 900$ m and the number of grid points is $80 \times 80 \times 60$. The CBL is capped by a thermally insulated no-slip rigid lid. The temperature of 300 K over the entire domain is used as the initial condition. The simulations start with the mixed layer at rest. To facilitate the growth of convective turbulence, small random disturbances are added to the initial temperature and velocity fields in the lower part of the mixed layer, and the subgrid-scale turbulence energy is set to a small value. The model is then run for several large eddy turnover times, defined as $\tau_* = hw_*^{-1}$, at which point the sampling of three-dimensional fields is started. The spinup time is $6\tau_*$ in case I and $4\tau_*$ in case II.

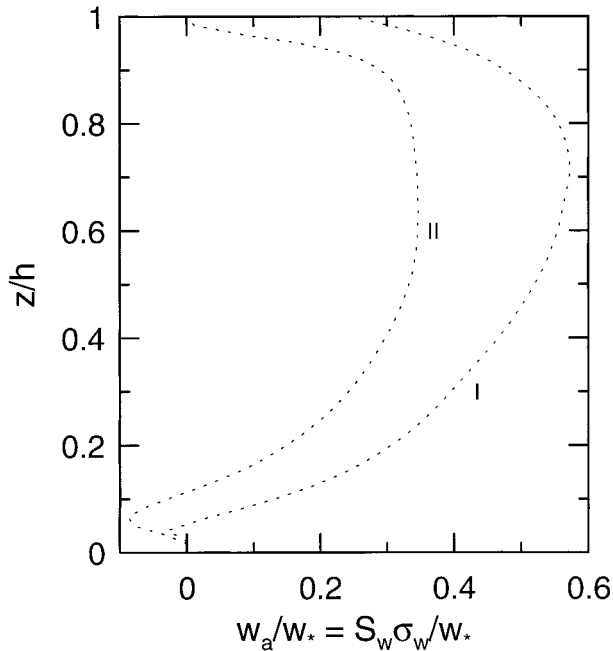


FIG. 2. LEST advection velocity w_a , Eq. (19), calculated from LES runs I and II.

Turbulent statistics discussed below are built by means of averaging over horizontal planes and over a number of recorded time steps (40 and 60 equidistant samples in cases I and II, respectively) as an approximation to the ensemble average. The sampling period covers about 12 large eddy turnover times. Only resolved-scale fields are used to compute the third-order moments since the subgrid-scale contribution is not available from our LES data. All curves in figures are normalized with the convective length h , velocity w_* , and temperature θ_* scales.

The LEST advection velocity w_a is shown in Fig. 2. It increases away from the surface, having a maximum above the CBL midplane. The spurious negative values of w_a in the near vicinity of the underlying surface are caused by inability of the LES model to appropriately handle the surface layer. The major concern in the present study, however, is the bulk of the CBL. Here, results from LES are hardly deteriorated by the above deficiency (see Schmidt and Schumann 1989).

Figure 3 compares the LES flux of flux of potential temperature, $\overline{w'^2\theta'}$, with its approximation through Eq. (25) taking $C_\theta = 1$ and $C_k = 0.1$. The turbulent diffusivity $K_{w\theta}$ is computed as $0.2\tau\sigma_w^2$, where the commonly accepted value of the dimensionless coefficient (0.2) is taken. The estimate of $C_\theta = 1$ follows from the bimodal bottom-up-top-down turbulence model discussed above, Eqs. (20)–(23). The same value of $C_\theta = 1$ is the maximum allowable value that obeys the realizability conditions for the other limiting case, when the quasi-normal approximation is used (see appendix A).

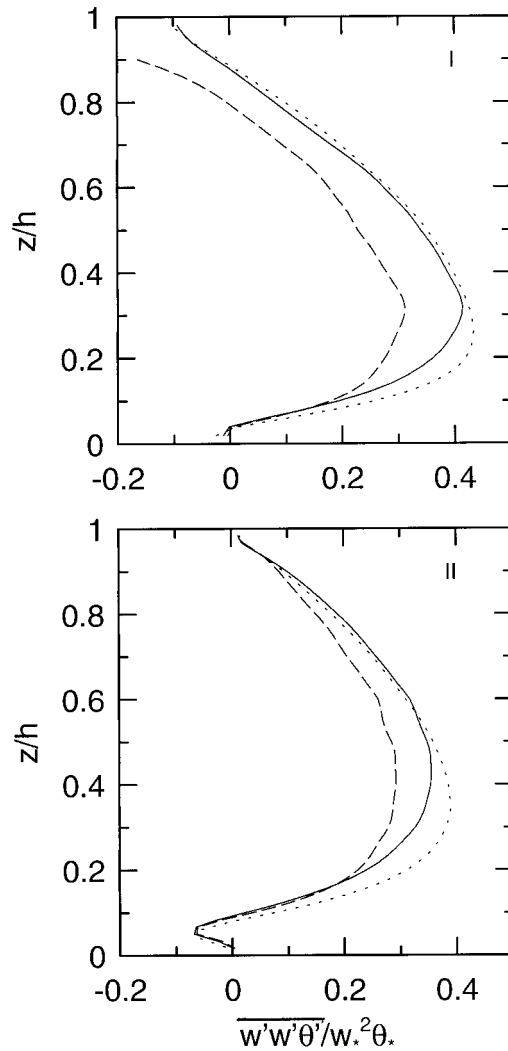


FIG. 3. Vertical profile of the flux of flux of potential temperature. Dotted lines are data from LES runs I and II; solid lines are computed from Eq. (25) with $C_\theta = 1$ and $C_k = 0.1$; and dashed lines from the quasi-normal approximation, Eq. (24).

The estimate of $C_k = 0.1$ is obtained by fitting the LES data by eye. In doing so, only one significant digit is kept, which is consistent with the accuracy of the other empirical constants. As seen from Fig. 3, in both cases the proposed parameterization for the third-order moment fits LES data well over most of the CBL. The flux of flux of potential temperature calculated from the quasi-normal approximation, Eq. (24), is also shown for comparison. Here, in both cases, $\overline{w'^2\theta'}$ is underestimated in mid-CBL. In case I with strong capping inversion, quasi-normal approximation strongly overestimates $\overline{w'^2\theta'}$ near the CBL top where the temperature gradient is strong.

The above analysis suggests empirical (LES) estimates

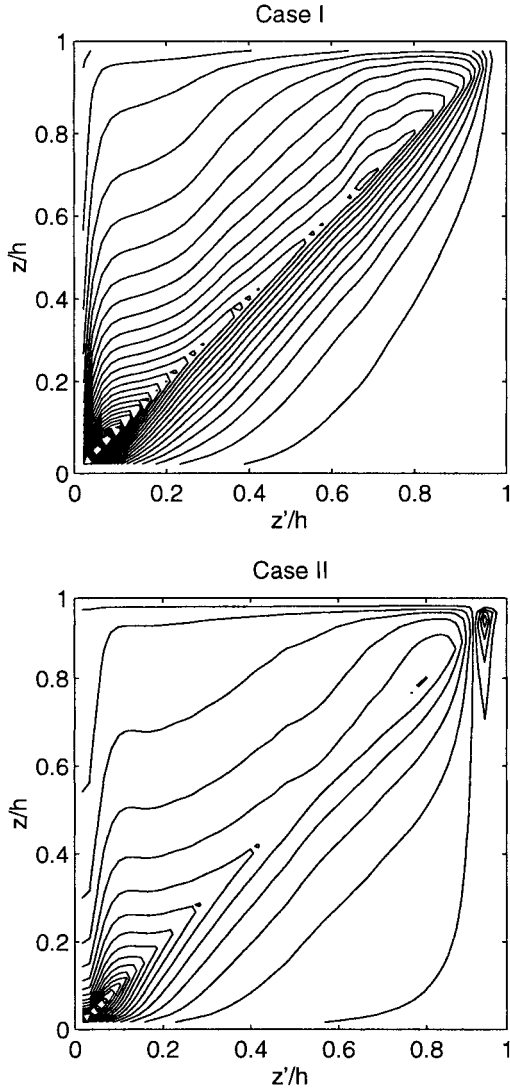


FIG. 4. Dimensionless Green functions $G(z, z')$, Eqs. (29)–(33), normalized with the CBL depth. The minimum and maximum values are -0.1 and 5.8 in case I, and -1.8 and 9.8 in case II. Contour lines (30 in each case) are equally spaced.

$$c_6 = 3, \quad c_7 = 0.4, \quad C_k = 0.1, \quad C_\theta = 1. \quad (26)$$

These values of dimensionless constants are used in further calculations shown in Figs. 4–7.

5. Flux transfer equation for potential temperature

a. Nonlocal integral closure

Employing our turbulent advection plus diffusion parameterization for the flux of flux of potential temperature, Eq. (25), together with conventional parameterization for the pressure gradient–temperature covariance, Eq. (10), the steady-state version of the potential temperature flux budget equation, Eq. (3), reads

$$\begin{aligned} \frac{\partial}{\partial z} K_{w\theta} \frac{\partial}{\partial z} \overline{w'\theta'} - C_\theta w_a \frac{\partial}{\partial z} \overline{w'\theta'} - \left(C_\theta \frac{\partial w_a}{\partial z} + \frac{1}{\tau_p} \right) \overline{w'\theta'} \\ = -(1 - c_7) \beta \sigma_\theta^2 + \sigma_w^2 \frac{\partial \Theta}{\partial z} - C_k \frac{\partial}{\partial z} \left(w_a K_{w\theta} \frac{\partial \Theta}{\partial z} \right). \end{aligned} \quad (27)$$

The first and the second terms on the lhs of Eq. (27) represent vertical transport of $\overline{w'\theta'}$ due to the down-gradient flux diffusion and due to the flux advection, respectively. The third term on the lhs may be referred to as the flux decay term as its main part, $\overline{w'\theta'}/\tau_p$, originates from the pressure gradient–potential temperature covariance, the sink term in the flux budget equation. A correction to the relaxation timescale occurs due to vertical changes of the LEST velocity. The rhs of Eq. (27) includes, from left to right, the production of the potential temperature flux by the buoyancy forces partially offset by buoyancy contribution to the pressure gradient–potential temperature covariance, the flux production/destruction due to the vertical gradient of mean potential temperature, and a correction term that originates from our parameterization of the third-order turbulent transport. The expression on the rhs of Eq. (27) could be loosely referred to as the source function.

It is worth mentioning that Eq. (10) for the pressure gradient–potential temperature covariance, although applies well to the CBL interior, may not be accurate near the boundaries. As pointed out by Moeng and Wyngaard (1986), the coefficient c_7 depends on the stability and structure of the inversion layer at the CBL top. As the major concern of the present study is nonlocal transport and consequently the third moment describing the flux of flux of potential temperature, we accept this deficiency and employ Eq. (10) with $c_6 = 3$ and $c_7 = 0.4$ throughout the CBL. The errors resulting from poor parameterization of the pressure term will manifest themselves in the expression of the source function on the rhs of Eq. (27).

We assume that all parameters involved are known functions of vertical coordinate z . In other words, we perform a diagnostic test of the proposed closure model. Using LES data to specify the dependence on z of both the rhs of Eq. (27) and the coefficients on the lhs of Eq. (27), we examine the ability of the model to reproduce a well-known linear profile of the potential temperature flux in the CBL.

As seen from Eq. (27), our turbulent advection plus diffusion parameterization introduces a correction to the relaxation timescale τ_p due to vertical changes of the LEST advection velocity w_a . This explains the fact that the combination that appears in the flux budget equation as an effective relaxation timescale, namely,

$$\tau_r = \frac{\tau_p}{1 + C_\theta \tau_p \partial w_a / \partial z}, \quad (28)$$

can be essentially different from the turbulence energy dissipation timescale τ , Eq. (11).

The boundary conditions for Eq. (27) are

$$\overline{w'\theta'} = \overline{w'\theta'}_0 \quad \text{at } z = 0, \quad (29)$$

$$\overline{w'\theta'} = \overline{w'\theta'}_h \quad \text{at } z = h, \quad (30)$$

where the heat flux due to entrainment, $\overline{w'\theta'}_h$, should be specified at the CBL top. Using this upper boundary condition we limit our closure model to the CBL interior. The heat transport in the inversion capping of the CBL is a separate problem beyond the scope of the present study.

Since Eq. (27) is a linear differential equation for $\overline{w'\theta'}$, the solution to the equation subject to boundary conditions (29) and (30) is given in terms of the Green function, namely,

$$\begin{aligned} \overline{w'\theta'} = - \int_0^h \tau_r \left[\sigma_w^2 \frac{\partial \Theta}{\partial z'} - (1 - c_7) \beta \sigma_\theta^2 \right. \\ \left. - C_k \frac{\partial}{\partial z'} \left(w_a K_{w\theta} \frac{\partial \Theta}{\partial z'} \right) \right] G(z, z') dz'. \end{aligned} \quad (31)$$

The Green function $G(z, z')$ is the solution to the equation

$$LG(z, z') = \delta(z - z'), \quad (32)$$

holding the boundary conditions, Eqs. (29) and (30), where the linear operator L is

$$L = \tau_r \left(\frac{\partial}{\partial z} K_{w\theta} \frac{\partial}{\partial z} - C_\theta w_a \frac{\partial}{\partial z} \right) - 1. \quad (33)$$

The Green function computed from the LES runs I and II (see section 4) is shown in Fig. 4.

In Fig. 5 LES data are employed to test the proposed parameterization for the potential temperature flux $\overline{w'\theta'}$, Eq. (31). Good correspondence between the model predictions and LES data is achieved taking $C_\theta = 1$ and $C_k = 0.1$. This indicates the non-Gaussian nature of convective turbulence. The Gaussian version of Eq. (31) (taking $C_\theta = 1/2$ and $C_k = 1/2$) and the purely diffusion version (taking $C_\theta = C_k = 0$) show worse results.

b. Decomposition into local and nonlocal components

Equation (31) is nothing but an integral generally nonlocal turbulence closure. Here, the values of the Green function $G(z, z')$ at the diagonal $z = z'$ characterize the local transport and the values at $z \neq z'$ the nonlocal transport. Equation (31) presents a convenient tool for analyzing various contributions to the vertical flux of potential temperature.

Thus, assuming decomposition

$$G(z, z') = \delta(z - z') + G_0(z, z'), \quad (34)$$

a number of earlier closure schemes are derived from Eq. (31). To classify local schemes, we set $G_0(z, z') \equiv 0$, which immediately results in Eq. (2) with the eddy

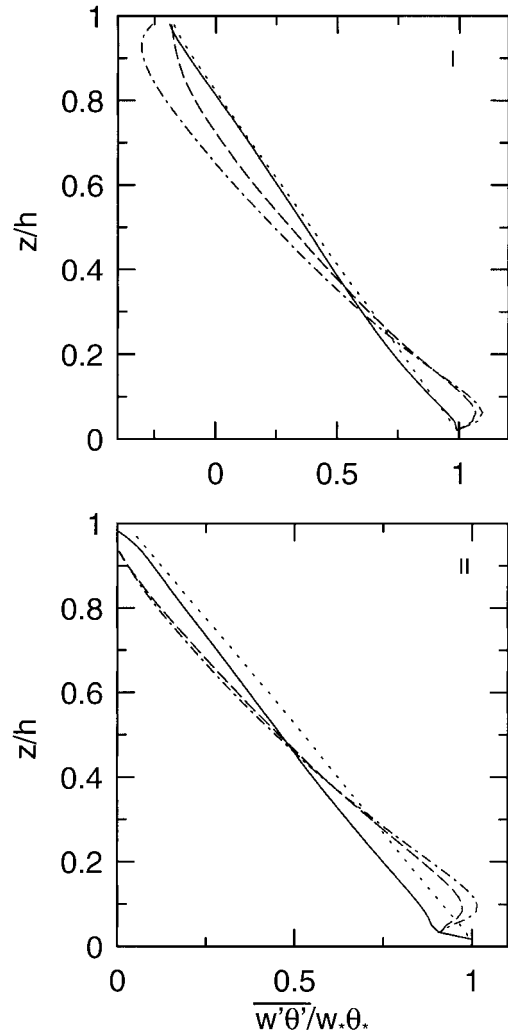


FIG. 5. Vertical profile of the potential temperature flux, $\overline{w'\theta'}$, in cases I and II. Dotted lines show LES data. Solid lines show our nonlocal closure model, Eq. (31) [or Eqs. (27)–(30)], with $C_\theta = 1$ and $C_k = 0.1$. Dashed and dot-dashed lines show the Gaussian model, Eq. (31) with $C_\theta = 1/2$ and $C_k = 1/2$, and the diffusion model, Eq. (31) with $C_\theta = C_k = 0$.

diffusivity K_H and the nongradient correction γ_H given by

$$\begin{aligned} K_H &= \frac{\tau_p \sigma_w^2}{1 + C_\theta \tau_p \partial w_a / \partial z}, \\ \gamma_H &= \frac{(1 - c_7) \beta \sigma_\theta^2}{\sigma_w^2} + \frac{C_k}{\sigma_w^2} \frac{\partial}{\partial z} \left(w_a K_{w\theta} \frac{\partial \Theta}{\partial z} \right). \end{aligned} \quad (35)$$

This generalized local parameterization includes

- 1) downgradient approximation, Eq. (1), taking $C_\theta = 0$, $C_k = 0$, and $c_7 = 1$;
- 2) a format similar to the Deardorff (1972) and the Troen and Mahrt (1986) countergradient correction, Eq. (5), taking $C_\theta = 0$, $C_k = 0$ and $0 \leq c_7 < 1$ (the

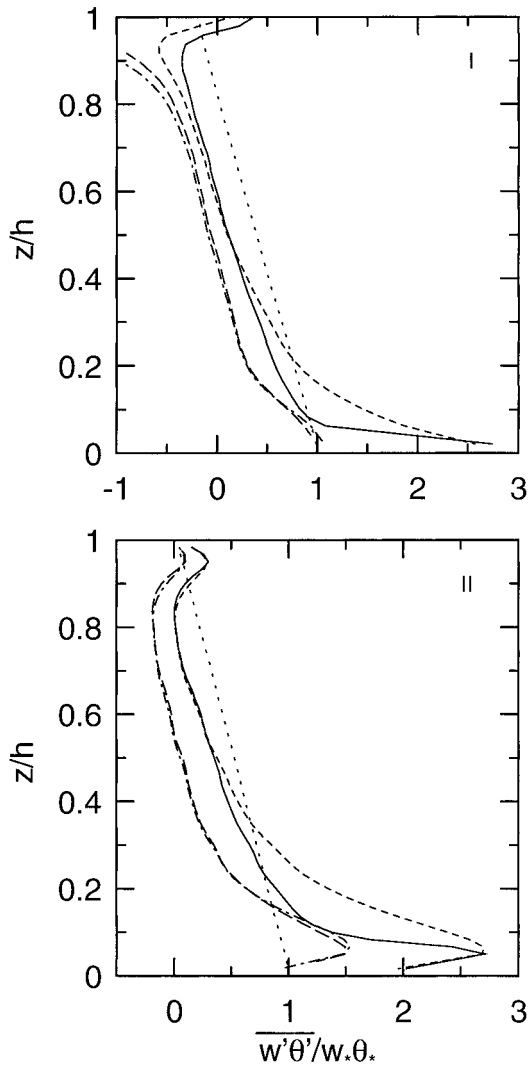


FIG. 6. Vertical profiles of the potential temperature flux in cases I and II computed diagnostically from different local closures using LES profiles of mean temperature and turbulence parameters involved. Dot-dashed lines show the downgradient approximation, Eq. (1); short dashed lines the Deardorff countergradient correction closure, Eq. (5); long dashed lines the Wyngaard and Weil (1991) nongradient closure, Eq. (15); and solid lines the generalized local closure, Eqs. (2) and (35) with $C_\theta = 1$ and $C_k = 0.1$. Dotted lines show the reference profiles calculated immediately from LES.

- Troen and Mahrt formulation further assumes that $\beta\sigma_w^2/\sigma_w^2$ is z independent); and
- 3) nongradient transport asymmetry formulation principally similar to the Wyngaard and Weil (1991) Eq. (15), taking $C_\theta = 0$, $C_k \neq 0$, and $c_7 = 1$.

Figure 6 shows results from diagnostic evaluation of the above local turbulence closures against data from our LES runs I and II. To attain these ends, mean potential temperature Θ and turbulence parameters that appear in the parameterizations involved, σ_w^2 , $\beta\sigma_\theta^2$, $K_{w\theta}$,

and w_a , are taken immediately from LES. As the basic earlier local closures are particular cases of Eqs. (2) and (35), the curves in Fig. 6 present different versions of the above equations. The reference “empirical” flux profiles are taken from LES.

As seen from the figure, the downgradient approximation overestimates $\overline{w'\theta'}$ in the surface layer and underestimates it in the CBL interior. Since the Deardorff correction is positive, it improves the approximation in the upper two-thirds of CBL but makes it worse in the lower portion of the layer. The generalized local “advection plus diffusion” formulation is close to the Deardorff closure in the CBL interior. In the lower portion of the CBL it performs better, except for the near vicinity of the surface where it overestimates $\overline{w'\theta'}$. By and large this parameterization, Eqs. (2) and (35) with $C_\theta = 1$ and $C_k = 0.1$, seems to perform slightly better than other local closures although, generally speaking, all of them leave much to be desired.

Needless to say, Eq. (34) allows one to decompose the flux $\overline{w'\theta'}$ into the local-transport and nonlocal-transport contributions given by $\overline{w'\theta'}_{[\text{Eqs. (2),(35)]}$ and $\overline{w'\theta'}_{[\text{Eq. (31)]} - \overline{w'\theta'}_{[\text{Eqs. (2),(35)]}$, respectively. To put it differently, it provides a mathematically rigorous procedure for the Frech and Mahrt (1995) decomposition, Eq. (13).

c. Decomposition into bottom-up and top-down components

We employ the following representation of the Green function:

$$G(z, z') = G_b(z, z') + G_t(z, z'), \quad (36)$$

where $G_b(z, z')$ is the contribution to $G(z, z')$ from below the diagonal $z = z'$ (including the diagonal itself) that accounts for the lower boundary condition (29), and $G_t(z, z')$ is the contribution to $G(z, z')$ from above the diagonal $z = z'$ that accounts for the upper boundary condition (30). Then the potential temperature flux immediately decomposes into two parts,

$$\overline{w'\theta'} = \overline{w'\theta'_b} + \overline{w'\theta'_t}, \quad (37)$$

calculated from Eq. (31) with $G(z, z')$ replaced by $G_b(z, z')$ and $G_t(z, z')$, respectively. Equations (36) and (37) equip the Wyngaard concept of the bottom-up and top-down diffusion with a mathematically rigorous algorithm for the decomposition.

Figure 7 shows the modeled potential temperature flux ($\overline{w'\theta'}$; solid lines) together with its bottom-up (b) and top-down (t) components ($\overline{w'\theta'_b}$ and $\overline{w'\theta'_t}$; dashed and dotted lines, respectively) specified using the Green-function formulation, Eqs. (36) and (37). Here, the b component dominates since the driving force for convection is the bottom heating.

An important point is that vertical profiles of both b - and t -components are essentially nonlinear even though the total flux decreases nearly linearly with height. By

this means our Green-function decomposition differs from conventional heuristic bottom-up–top-down decomposition, which adopts linear b - and t -flux profiles as a sort of axiom. In particular, our formulation suggests essentially nonzero top-down flux $\overline{w'\theta'_t}$, in nonpenetrative convection (our run II with no entrainment at the CBL top, $\overline{w'\theta'_h} = 0$). We remember that conventional formulation scales $\overline{w'\theta'_t}$ with $\overline{w'\theta'_h}$ and therefore suggests $\overline{w'\theta'_t} = 0$ in the regime in question. This implies no contribution to total transport from downdrafts, which seems unrealistic.

6. Conclusions

An advanced nonlocal turbulence closure scheme is developed for the potential temperature flux in convective boundary layers. It provides better understanding and improved parameterization of the third-order transport in the budget equation for the potential temperature flux.

As an alternative to traditional turbulence diffusion parameterization, a new turbulence advection plus diffusion parameterization for the flux of flux of potential temperature, $\overline{w'^2\theta'}$, is developed. In the CBL interior (away from the underlying surface and the inversion layer) the flux in question, $\overline{w'^2\theta'}$, is shown to be proportional to the second-order flux involved, $\overline{w'\theta'}$, multiplied by a large eddy skewed-turbulence advection velocity (LEST advection velocity), w_a , Eq. (19). To embrace the entire convective zone, an interpolation between this turbulence advection formulation and a version of turbulence diffusion formulation is derived. Comparison of the resulting parameterization, Eq. (25), with LES data shows good agreement throughout the CBL.

Using the proposed parameterization for the third-order flux $\overline{w'^2\theta'}$ together with traditional formulation for the pressure gradient–temperature covariance results in a nonlocal closure, Eq. (27), for the second-order flux $\overline{w'\theta'}$. The solution to Eq. (27) in terms of the Green function, Eq. (31), provides a convenient tool to distinguish between local and nonlocal contributions to $\overline{w'\theta'}$ and to classify a number of earlier turbulence closure schemes. These include the simplest downgradient approximation, some known countergradient and nongradient correction formulations and a nonlocal integral closure.

The proposed nonlocal turbulence closure is diagnostically tested against LES data. The model fairly accurately reproduces practically linear vertical profiles of the potential temperature flux in the CBL. It can be adjusted to practical applications in numerical models, provided that the turbulence parameters involved, σ_w , σ_θ , τ , and S_w , are known. The latter can be either calculated from the appropriate budget equations or taken as given empirical functions, for example, those specified with the aid of revised versions of the shear-free-convection scaling (Sorbjan 1988, 1989; Hartmann

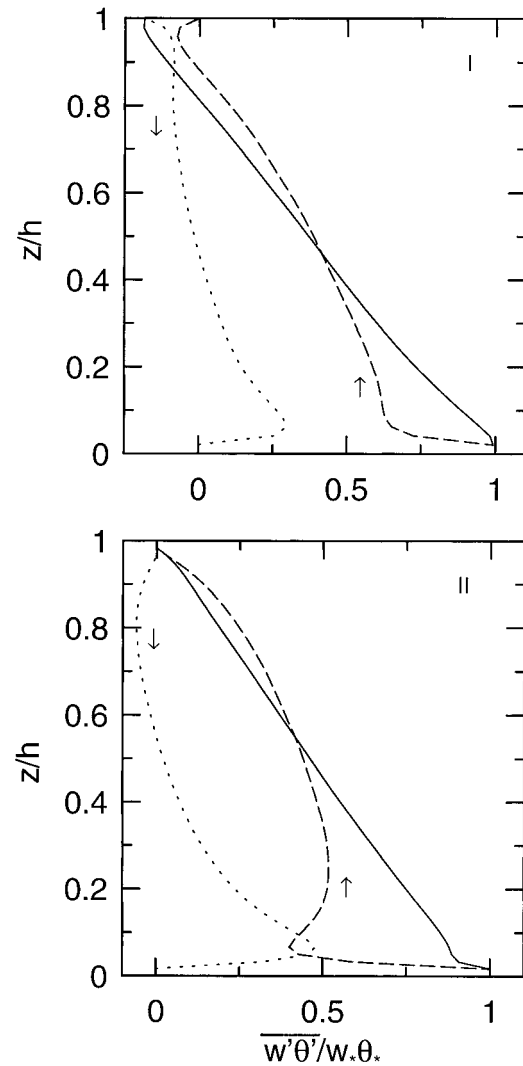


FIG. 7. Decomposition of the potential temperature flux $\overline{w'\theta'}$ employing integral closure, Eq. (31), with decomposed Green function, Eq. (36), in cases I and II. Total flux is shown by solid lines, the bottom-up component $\overline{w'\theta'_b}$ by dashed lines, and the top-down component $\overline{w'\theta'_t}$ by dotted lines.

1990) and generalized scaling for convective sheared flows (Zilitinkevich 1994).

The proposed Green-function formulation for the potential temperature flux provides mathematically rigorous decomposition of the flux in question into the bottom-up and top-down components. These components are shown to be essentially nonlinear functions of height within the well-mixed layer, in striking contrast to conventional assumption of linearity. Moreover, the proposed decomposition exhibits essentially nonzero top-down flux in the nonpenetrative convection regime, once again contrary to traditional routes. It puts us on the right track for development of a rigorous bottom-up–top-down decomposition for other statistics and for

revision of scaling formulations for both shear-free and sheared convection.

Physical ideas underlying our approach diverge from classic turbulence closure philosophy, according to which a flux in question is expressed as a function of turbulence moments of the same or the lower order. Our parameterization for the potential temperature flux $\overline{w'\theta'}$ (the second-order moment) involves not only the first-order moment (potential temperature gradient $\partial\Theta/\partial z$) and the second-order moments (rms vertical velocity and temperature, σ_w and σ_θ), but also the third-order moment, namely, the vertical velocity triple correlation $\overline{w'^3}$, or alternatively the vertical velocity skewness [cf. the earlier Wyngaard and Weil (1991) formulation for the passive scalar transport that includes the skewness in the expression of the second-order turbulent flux].

The proposed advection plus diffusion turbulence closure is likely to be applicable also to the passive scalar transport in near-neutral skewed turbulence. In that case, taking $\beta = 0$, that is, considering the quantity θ in Eqs. (27), (29), and (30) as a passive scalar, our derivation basically remains in force. Moreover, an attempt could be made to apply a similar approach, employing an advection plus diffusion closure, to the momentum transport [for earlier nonlocal momentum-transport models see Lykossov (1992)].

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APPENDIX A

Realizability Conditions

We consider the realizability conditions (see Andre 1976; Schumann 1977) for the turbulence advection parameterization for the flux of flux of potential temper-

ature, Eqs. (18) and (19). The Schwartz inequality applied to the third-order moment, $\overline{w'^2\theta'}$, and the second-order moment, $\overline{w'\theta'}$, reads

$$(\overline{w'^2\theta'})^2 \leq \min[(\overline{w'\theta'})^2 \overline{w'^2}, \overline{w'^4} \overline{\theta'^2}], \quad (\text{A1})$$

$$|\overline{w'\theta'}| \leq \sigma_w \sigma_\theta. \quad (\text{A2})$$

Applying the quasi-normal Gaussian approximation,

$$\overline{\alpha'\beta'\gamma'\delta'} = \overline{\alpha'\beta'}\overline{\gamma'\delta'} + \overline{\alpha'\gamma'}\overline{\beta'\delta'} + \overline{\alpha'\delta'}\overline{\beta'\gamma'}, \quad (\text{A3})$$

to the fourth-order covariances on the rhs of Eq. (A1) yields

$$|\overline{w'^2\theta}| \leq \min[\sigma_w \sqrt{\sigma_w^2 \sigma_\theta^2 + 2(\overline{w'\theta'})^2}, \sqrt{3} \sigma_w^2 \sigma_\theta]. \quad (\text{A4})$$

Then substituting $\overline{w'\theta'}$ from Eq. (A2) yields

$$|\overline{w'^2\theta'}| \leq \tilde{C}_\theta \sigma_w |\overline{w'\theta'}|, \quad \tilde{C}_\theta = \sqrt{2 + 1/c^2}, \quad (\text{A5})$$

where $c = \overline{w'\theta'}/(\sigma_w \sigma_\theta) \leq 1$ is the correlation coefficient. The same procedure for $\overline{w'^2\theta'}$ parameterized through Eq. (18) yields

$$|\overline{w'^2\theta'}| \leq \sqrt{3} C_\theta \sigma_w |\overline{w'\theta'}|. \quad (\text{A6})$$

Taking $c = 1$, the minimum of the rhs of the first formula in Eq. (A5) is $\sqrt{3} \sigma_w |\overline{w'\theta'}|$. Then the strongest constraint, namely, that the lhs of Eq. (A6) does not exceed the above minimum, yields $C_\theta \leq 1$.

APPENDIX B

Heuristic Arguments in Support of the Advection Plus Diffusion Turbulence Closure, Suggested by the Third-Order-Moment Budget Equations

We express the fourth-order moments in the budget equations for the third-order moments $\overline{w'^2\theta'}$, $\overline{w'\theta'^2}$, $\overline{w'^3}$, and $\overline{\theta'^3}$ through the second-order moments using quasi-normal approximation and apply a return-to-isotropy approximation similar to Eq. (10) for the pressure terms. In the steady state, the resulting equations read (e.g., Moeng and Randall 1984; Canuto et al. 1994)

$$\begin{aligned} c_8 \tau^{-1} \overline{w'^2\theta'} - 2 \left(1 - \frac{2}{3} c_{11} \right) \overline{\beta w'\theta'^2} + \overline{w'\theta'} \frac{\partial \overline{w'^2}}{\partial z} \\ = - \left(\overline{w'^3} \frac{\partial \Theta}{\partial z} + 2 \overline{w'^2} \frac{\partial \overline{w'\theta'}}{\partial z} \right), \end{aligned} \quad (\text{B1})$$

$$\begin{aligned} 2 \overline{w'^2\theta'} \frac{\partial \Theta}{\partial z} + c_8 \tau^{-1} \overline{w'\theta'^2} - (1 - c_{11}) \beta \overline{\theta'^3} \\ = - \left(2 \overline{w'\theta'} \frac{\partial \overline{w'\theta'}}{\partial z} + \overline{w'^2} \frac{\partial \overline{\theta'^2}}{\partial z} \right), \end{aligned} \quad (\text{B2})$$

$$3 \overline{w'\theta'^2} \frac{\partial \Theta}{\partial z} + c_{10} \tau^{-1} \overline{\theta'^3} = -3 \overline{w'\theta'} \frac{\partial \overline{\theta'^2}}{\partial z}, \quad (\text{B3})$$

$$3(1 - c_{11}) \overline{\beta w'\theta'^2} - 3 \overline{w'^2} \frac{\partial \overline{w'^2}}{\partial z} = c_8 \tau^{-1} \overline{w'^3}, \quad (\text{B4})$$

where c_8 , c_{10} , and c_{11} are positive dimensionless constants ($c_{11} < 1$). In the conventional derivation of diffusion-type closure models, Eqs. (B1)–(B4) are solved for the four third-order moments that are thus expressed in terms of the second-order moments and mean profiles. By contrast, we keep the third moment $\overline{w'^3}$ as a basic governing parameter and solve Eqs. (B1)–(B4) for the three *third-order* moments, $\overline{w'^2\theta'}$, $\overline{w'\theta'^2}$, and $\overline{\theta'^3}$, and the gradient of the *second-order* moment, $\partial\overline{w'^2}/\partial z$. This yields the expression of the flux of flux of potential temperature,

$$\begin{aligned} \overline{w'^2\theta'} = & -\alpha_1 K_{w\theta} \frac{\partial\overline{w'\theta'}}{\partial z} - \alpha_2 \beta \tau K_{w\theta} \frac{\partial\overline{\theta'^2}}{\partial z} \\ & + \frac{1}{3} \eta_1 \frac{\overline{w'^3}}{\overline{w'^2}} \overline{w'\theta'} - \frac{1}{2} \eta_1 \tau \overline{w'^3} \frac{\partial\Theta}{\partial z}, \end{aligned} \quad (\text{B5})$$

with the eddy diffusivity $K_{w\theta}$ given by

$$K_{w\theta} = 2\tau\sigma_w^2/c_8, \quad (\text{B6})$$

where α_1 , α_2 , and η_1 are functions of two dimensionless combinations, $R_1 = \tau^2 \beta \partial\Theta/\partial z$ and $R_2 = \tau \beta \overline{w'\theta'}/\sigma_w^2$,

$$\alpha_1 = \eta_1 \left[1 + \frac{2}{c_8} \eta_2 R_2 \right], \quad (\text{B7})$$

$$\alpha_2 = \frac{\eta_1 \eta_2}{c_8} \left[1 + \frac{3(1 - c_{11})}{c_{10}} R_2 \right], \quad (\text{B8})$$

$$\eta_1 = \left[1 + \left(\frac{2}{c_8} \right)^2 \eta_2 R_1 + \frac{1 - c_{11}}{c_8} R_2 \right]^{-1}, \quad (\text{B9})$$

and η_2 is one more function

$$\eta_2 = \left(1 - \frac{2}{3} c_{11} \right) \left[1 + \frac{3(1 - c_{11})}{c_8 c_{10}} R_1 \right]^{-1}. \quad (\text{B10})$$

Here, $\sqrt{R_1}$ is the ratio of the dissipation timescale τ to the buoyancy timescale N^{-1} ($N^2 = \beta \partial\Theta/\partial z$ being the squared buoyancy frequency), and R_2 is the ratio of the buoyant diffusivity $\tau^2 \beta \overline{w'\theta'}$ to the mechanical diffusivity $\tau\sigma_w^2$.

In the CBL interior, the mean potential temperature gradient $\partial\Theta/\partial z$ is small. Hence, $R_1 \approx 0$, and the above functions depend only on R_2 . As long as R_2 is also small, Eqs. (B7)–(B10) reduce to $\alpha_1 \approx 1$, $\alpha_2 \approx 0.1$, $\eta_1 \approx 1$, and $\eta_2 \approx 0.9$ (adopting conventional values of $c_8 = 8$ and $c_{11} = 0.2$; see Moeng and Randall 1984). Provided that vertical gradient of the potential temperature variance $\partial\overline{\theta'^2}/\partial z$ is small, Eq. (B5) reduces to Eq. (24).

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