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ABSTRACT

The energy and flux budget (EFB) closure theory for a passive scalar (non-buoyant and non-inertial particles or gaseous admixtures) is developed for stably stratified turbulence. The physical background of the EFB turbulence closures is based on the budget equations for the turbulent kinetic and potential energies and turbulent fluxes of momentum and buoyancy as well as the turbulent flux of particles. The EFB turbulence closure is designed for stratified geophysical flows from neutral to very stable stratification, and it implies that turbulence is maintained by the velocity shear at any stratification. In a steady-state, expressions for the turbulent flux of the passive scalar and the anisotropic non-symmetric turbulent diffusion tensor are derived, and universal flux Richardson number dependencies of the components of this tensor are obtained. The diagonal component in the vertical direction of the turbulent diffusion tensor is suppressed by strong stratification, while the diagonal components in the horizontal directions are not suppressed, but they are dominant in comparison with the other components of the turbulent diffusion tensor. This implies that any initially created strongly inhomogeneous particle cloud is evolved into a thin pancake in a horizontal plane with very slow increase in its thickness in the vertical direction. The turbulent Schmidt number (the ratio of the eddy viscosity and the vertical turbulent diffusivity of the passive scalar) linearly increases with the gradient Richardson number. The physics of such a behavior is related to the buoyancy force that causes a correlation between fluctuations of the potential temperature and the particle number density. This correlation that is proportional to the product of the vertical turbulent particle flux and the vertical gradient of the mean potential temperature reduces the vertical turbulent particle flux. Considering the applications of these results to the atmospheric boundary-layer turbulence, the theoretical relationships are derived, which allows us to determine the turbulent diffusion tensor as a function of the vertical coordinate measured in the units of the local Obukhov length scale. The obtained relations are potentially useful in modeling applications of particle dispersion in the atmospheric boundary-layer turbulence and free atmosphere turbulence.

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I. INTRODUCTION

Turbulence and the associated turbulent transport of the passive scalar have been systematically investigated for more than a hundred years in theoretical, experimental, and numerical studies.^{1–8} However, some fundamental questions remain. This is particularly true in applications such as geophysics and astrophysics, where the governing parameter values are too large to be modeled either experimentally or numerically.

The classical theory of atmospheric turbulence implies that the turbulent flux of any quantity is a product of a mean gradient of the quantity and a turbulent-exchange coefficient (e.g., eddy viscosity, eddy diffusivity, etc.).^{1,2,9,10} This corresponds to a down-gradient

transport where the turbulent-exchange coefficients are proportional to the density of the turbulent kinetic energy multiplied by the turbulent timescale. This has been originally formulated for neutrally stratified turbulence.^{9,10}

Many turbulence closure models of stratified turbulence in meteorological applications^{1,2,11} have been based only on the density of the turbulent kinetic energy equation, not considering an evolution of the density of the turbulent potential energy proportional to the second moment of potential temperature fluctuations. In stable stratification, such turbulence closure models have resulted in the erroneous conclusion that shear-generated turbulence inevitably decays and that the flow becomes laminar in “supercritical” stratifications (at the gradient

Richardson number exceeding some critical values),^{12,13} where the gradient Richardson number is the ratio of the squared Brunt-Väisälä frequency (proportional to the gradient of the mean potential temperature) to the squared mean velocity shear.

Contradictions of this conclusion via the well-documented universal existence of turbulence under strongly supercritical conditions typical of the free atmosphere and the deep ocean^{14–22} have been attributed to some unknown mechanisms and, in practical applications, mastered heuristically.^{21–23} Numerous alternative turbulence closures in stratified turbulence have been formulated using the budget equations for various turbulent parameters (in addition to the density of the turbulent kinetic energy) together with heuristic hypotheses and empirical relationships.^{11,24}

As an alternative, the energy and flux budget (EFB) theory of turbulence closure for stably stratified dry atmospheric flows has been recently developed.^{25–30} In agreement with the wide experimental evidence, the EFB theory shows that high-Reynolds-number turbulence is maintained by shear in any stratification, and the “critical Richardson number,” treated many years as a threshold between the turbulent and laminar regimes, actually separates two turbulent regimes, namely, the strong turbulence typical of atmospheric boundary layers and the weak three-dimensional turbulence typical of the free atmosphere or deep ocean, characterized by a strong decrease in the heat transfer in comparison to the momentum transfer. The EFB theory has been verified against scarce data from the atmospheric experiments, direct numerical simulations (DNS), large-eddy simulations (LES), and laboratory experiments relevant to the steady-state turbulence regime.^{25,26,29} Following the EFB closure, other turbulent closure models also do not imply a critical Richardson number.^{31–40}

In stably stratified turbulence, large-scale internal gravity waves result in additional vertical turbulent flux of momentum and additional productions of the densities of the turbulent kinetic energy (TKE), turbulent potential energy (TPE), and turbulent flux of potential temperature.^{27,30} For the stationary, homogeneous regime, the EFB theory in the absence of the large-scale internal gravity waves (IGW) yields universal dependencies of the flux Richardson number, the turbulent Prandtl number, the ratio of TKE to TPE, and the normalized vertical turbulent fluxes of momentum and heat on the gradient Richardson number.^{25,29} Due to the large-scale IGW, these dependencies lose their universality. The maximal value of the flux Richardson number (universal constant 0.2–0.25 in the no-IGW regime) becomes strongly variable in the turbulence with large-scale IGW. In the vertically homogeneous stratification, the flux Richardson number increases with the increasing wave energy. In addition, the large-scale internal gravity waves reduce the anisotropy of turbulence. Predictions from this theory are consistent with available data from atmospheric and laboratory experiments, DNS and LES.^{27,30}

In the present study, we develop the energy and flux budget turbulence closure theory for a passive scalar (non-buoyant, non-inertial particles and gaseous admixtures) for stably stratified turbulence. We find that the vertical turbulent diffusion coefficient of the passive scalar is strongly reduced for large gradient Richardson numbers, and the turbulent Schmidt number (the ratio of the eddy viscosity and the vertical turbulent diffusivity of the passive scalar) linearly increases with the gradient Richardson number.

For atmospheric boundary-layer turbulence, we derive the theoretical relationships for the vertical profiles of the turbulent diffusion

tensor and the turbulent Schmidt number. This study can be useful in modeling applications for atmospheric boundary-layer turbulence and free atmosphere turbulence. For example, the transport of pollutants in the atmospheric turbulent flows is an important environmental problem (see Ref. 41–43 and references therein). In stratified flows, the turbulent Schmidt number increases with the level of stratification.^{44,45} This is consistent with the observation that stratification acts more effectively against mass diffusivity than against momentum diffusivity. In spite of many studies, there is still controversy about the proper parameterization of the turbulent Schmidt number for various environmental flows.^{44,46}

This paper is organized as follows: In Sec. II, we outline the EFB theory for turbulence, where we formulate governing equations for the energy and flux budget turbulence-closure theory for stably stratified turbulence and consider the steady-state and homogeneous regime of turbulence. In Sec. III, we develop the EFB theory for passive scalars, deriving the budget equation for the turbulent flux of particles, which yields the expression for the turbulent diffusion tensor. In Sec. IV, we consider the applications of the obtained results to the atmospheric boundary-layer turbulence and discuss the theoretical relationships potentially useful in modeling applications. Finally, conclusions are drawn in Sec. V. In the Appendix, we derive the budget equation for the correlation function for fluctuations of particle number density and temperature.

II. THE EFB THEORY FOR STABLY STRATIFIED TURBULENCE

In this study, we consider fully developed stably stratified turbulence for geophysical flows where typical vertical gradients of the mean velocity, potential temperature, and other variables are much larger than that of the horizontal gradients so that the direct effects of the mean-flow horizontal gradients on turbulent statistics are negligible. In such flows, vertical scales of motions are much smaller than horizontal scales, and the mean-flow vertical velocity is much smaller than the horizontal velocities. This implies that vertical turbulent transports are comparable with or even dominate the mean flow vertical advection, whereas the stream-wise horizontal turbulent transport is usually negligible compared to the horizontal advection.

In this section, we formulate the energy and flux budget (EFB) closure theory for stably stratified turbulence based on the budget equations for the densities of turbulent kinetic and potential energies and turbulent fluxes of momentum and heat. In our analysis, we use budget equations for the one-point second moments to develop a mean-field theory. We do not study small-scale structures of turbulence (i.e., higher moments for turbulent quantities and intermittency). In particular, we study large-scale long-term dynamics, i.e., we consider effects in the spatial scales, which are much larger than the integral scale of turbulence, and in timescales, which are much longer than the turbulent timescales.

A. Budget equations for turbulence

In the framework of the energy and flux budget turbulence theory,^{25,29} we use the budget equations for the density of turbulent kinetic energy (TKE) $E_K = \langle \mathbf{u}^2 \rangle / 2$, the intensity of potential temperature fluctuations $E_\theta = \langle \theta^2 \rangle / 2$, the turbulent flux $F_i = \langle u_i \theta \rangle$ of potential temperature, and the off diagonal components of the Reynolds stress $\tau_{iz} = \langle u_i u_z \rangle$ with $i = x, y$,

$$\frac{DE_K}{Dt} + \nabla_z \Phi_K = -\tau_{iz} \nabla_z \bar{U}_i + \beta F_z - \varepsilon_K, \quad (1)$$

$$\frac{DE_\theta}{Dt} + \nabla_z \Phi_\theta = -F_z \nabla_z \bar{\Theta} - \varepsilon_\theta, \quad (2)$$

$$\frac{\partial F_i}{\partial t} + \nabla_z \Phi_i^{(F)} = -\tau_{iz} \nabla_z \bar{\Theta} \delta_{i3} + 2\beta E_\theta \delta_{i3} - \frac{1}{\rho_0} \langle \theta \nabla_i p \rangle - F_z \nabla_z \bar{U}_i - \varepsilon_i^{(F)}, \quad (3)$$

$$\frac{D\tau_{iz}}{Dt} + \nabla_z \Phi_i^{(\tau)} = -2E_z \nabla_z \bar{U}_i - \varepsilon_i^{(\tau)}, \quad (4)$$

where $D/Dt = \partial/\partial t + \bar{\mathbf{u}} \cdot \nabla$, the fluid velocity $\bar{\mathbf{u}} + \mathbf{u}$ is characterized by the mean fluid velocity $\bar{\mathbf{U}}(z) = (\bar{U}_x, \bar{U}_y, 0)$ and fluctuations $\mathbf{u} = (u_x, u_y, u_z)$, $E_z = \langle u_z^2 \rangle / 2$ is the density of the vertical turbulent kinetic energy, $F_z = \langle u_z \theta \rangle$ is the vertical component of the turbulent heat flux, δ_{ij} is the Kronecker unit tensor, the angular brackets imply ensemble averaging, $\Theta = T(P_*/P)^{1-\gamma^{-1}}$ is the potential temperature, T and P are the fluid temperature and pressure with their reference values, T_* and P_* , respectively, $\gamma = c_p/c_v$ is the specific heat ratio, the potential temperature $\Theta = \bar{\Theta} + \theta$ is characterized by the mean potential temperature $\bar{\Theta}(z)$ and fluctuations θ , the fluid pressure $P = \bar{P} + p$ is characterized by the mean pressure \bar{P} and fluctuations p , $\beta = g/T_*$ is the buoyancy parameter, \mathbf{g} is the gravity acceleration, and ρ_0 is the fluid density. We use here the Boussinesq approximation.

The term $\Pi_K \equiv -\tau_{iz} \nabla_z \bar{U}_i = K_M S^2$ is the rate of energy production for the shear-produced turbulence, K_M is the turbulent viscosity, and $S = [(\nabla_z \bar{U}_x)^2 + (\nabla_z \bar{U}_y)^2]^{1/2}$ is the large-scale velocity shear. The terms Φ_K , Φ_θ , $\Phi_i^{(F)}$, and $\Phi_i^{(\tau)}$ include the third-order moments. In particular, $\Phi_K = \rho_0^{-1} \langle u_z p \rangle + (\langle u_z \mathbf{u}^2 \rangle - \nu \nabla_z \langle \mathbf{u}^2 \rangle) / 2$ determines the flux of E_K ; $\Phi_\theta = (\langle u_z \theta^2 \rangle - \kappa \nabla_z \langle \theta^2 \rangle) / 2$ describes the flux of E_θ ; $\Phi_i^{(F)} = \langle u_i u_z \theta \rangle - \nu \langle \theta (\nabla_z u_i) \rangle - \kappa \langle u_i (\nabla_z \theta) \rangle$ determines the flux of F_i ; and $\Phi_i^{(\tau)} = \langle u_i u_z^2 \rangle + \rho_0^{-1} \langle p u_i \rangle - \nu \nabla_z \tau_{iz}$ describes the flux of τ_{iz} .

The term $\varepsilon_K = \nu \langle (\nabla_j u_i)^2 \rangle$ is the dissipation rate of the density of the turbulent kinetic energy, $\varepsilon_\theta = \kappa \langle (\nabla \theta)^2 \rangle$ is the dissipation rate of the intensity of potential temperature fluctuations E_θ ; and $\varepsilon_i^{(F)} = (\nu + \kappa) \langle (\nabla_j u_i) (\nabla_j \theta) \rangle$ is the dissipation rate of the turbulent heat flux F_i , where ν is the kinematic viscosity of the fluid, and κ is the temperature diffusivity. The term $\varepsilon_i^{(\tau)} = \varepsilon_{iz}^{(\tau)} - \beta F_i - Q_{iz}$ in Eq. (4) is the “effective dissipation rate” of the off diagonal components of the Reynolds stress τ_{iz} , where $Q_{ij} = \rho_0^{-1} (\langle p \nabla_j u_i \rangle + \langle p \nabla_j u_i \rangle)$ and $\varepsilon_{iz}^{(\tau)} = 2\nu \langle (\nabla_j u_i) (\nabla_j u_z) \rangle$ are the molecular-viscosity dissipation rate (see below).^{25,29}

The first term, $-\tau_{iz} \nabla_z \bar{\Theta} \delta_{i3}$, in the right-hand side of Eq. (3) contributes to the traditional vertical turbulent flux of the potential temperature, which describes the classical gradient mechanism of the turbulent heat transfer. On the other hand, the second and third terms in the right-hand side of Eq. (3) describe a non-gradient contribution to the vertical turbulent flux of the potential temperature. In stably stratified flows, the gradient and non-gradient contributions to the vertical turbulent flux of potential temperature have opposite signs [see Eq. (7)]. This implies that the non-gradient contribution decreases the traditional gradient turbulent flux.

The budget equations for the components of the turbulent kinetic energies $E_\alpha = \langle u_\alpha^2 \rangle / 2$ along the x , y , and z directions can be written as follows:

$$\frac{DE_\alpha}{Dt} + \nabla_z \Phi_\alpha = -\tau_{\alpha z} \nabla_z \bar{U}_\alpha + \delta_{\alpha 3} \beta F_z + \frac{1}{2} Q_{\alpha\alpha} - \varepsilon_\alpha, \quad (5)$$

where $\alpha = x, y, z$, the term $\varepsilon_\alpha = \nu \langle (\nabla_j u_\alpha)^2 \rangle$ is the dissipation rate of the turbulent kinetic energy components E_α , and Φ_α determines the flux of E_α . Here, $\Phi_z = \rho_0^{-1} \langle u_z p \rangle + (\langle u_z^3 \rangle - \nu \nabla_z \langle u_z^2 \rangle) / 2$ and $\Phi_{x,y} = (\langle u_z u_{x,y}^2 \rangle - \nu \nabla_z \langle u_{x,y}^2 \rangle) / 2$. The terms $Q_{\alpha\alpha} = 2\rho_0^{-1} \langle p \nabla_\alpha u_\alpha \rangle$ are the diagonal terms of the tensor Q_{ij} . In Eq. (5), we do not apply the summation convention for the double Greek indices. Different aspects related to budget equations (1)–(5) have been discussed in a number of publications.^{25–30,47–50}

The density of turbulent potential energy (TPE) is determined by potential temperature fluctuations and is defined as $E_P = (\beta^2/N^2) E_\theta$, where $N^2 = \beta \nabla_z \bar{\Theta}$ with N being the Brunt-Väisälä frequency. The budget equation for the density of turbulent potential energy $E_P = (\beta^2/N^2) E_\theta$ reads as follows:

$$\frac{\partial E_P}{\partial t} + \nabla_z \Phi_P = -\beta F_z - \varepsilon_P, \quad (6)$$

where $-\beta F_z$ is the rate of the production of the turbulent potential energy density, $\Phi_P = (\beta^2/N^2) \Phi_\theta$ is the flux of E_P , and $\varepsilon_P = (\beta^2/N^2) \varepsilon_\theta$ is the dissipation rate of the density of the turbulent potential energy. Using Eqs. (1) and (5), we obtain the budget equation for the density of the total turbulent energy $E_T = E_K + E_P$ as^{25,29}

$$\frac{\partial E_T}{\partial t} + \nabla_z \Phi_T = -\tau_{iz} \nabla_z \bar{U}_i - \varepsilon_T, \quad (7)$$

where $\Phi_T = \Phi_K + \Phi_P$ is the flux of E_T and $\varepsilon_T = \varepsilon_K + \varepsilon_P$ is the dissipation rate of the density of the total turbulent energy.

B. Steady-state and homogeneous regime of turbulence

The discussed energy and flux budget turbulence closure theory for stably stratified flows assumes the following:

- The characteristic times of variations of the densities of the turbulent kinetic energy (TKE) E_K , the vertical and horizontal TKE E_x , the intensity of potential temperature fluctuations E_θ (and the turbulent potential energy E_P), the turbulent flux F_i of the potential temperature, and the turbulent flux τ_{iz} of momentum (i.e., the off diagonal components of the Reynolds stress) are much larger than the turbulent timescale. This allows us to obtain steady-state solutions of the budget equations (1)–(7) for TKE, TPE, TTE, F_i , E_α , and τ_{iz} for stably stratified turbulence.
- We neglect the divergence of the fluxes of TKE, TPE, E_α , F_i , and τ_{iz} for a steady-state homogeneous regime of stably stratified turbulence (i.e., we neglect the divergence of third-order moments).
- Dissipation rates of TKE, TPE, E_α , and F_i are expressed using the Kolmogorov hypothesis, i.e., $\varepsilon_K = E_K/t_T$, $\varepsilon_\theta = E_\theta/(C_p t_T)$, $\varepsilon_{\alpha\alpha}^{(\tau)} = E_\alpha/3t_T$, and $\varepsilon_i^{(F)} = F_i/(C_F t_T)$, where $t_T = \ell_0/E_K^{1/2}$ is the turbulent dissipation timescale, ℓ_0 is the integral scale of turbulence, and C_p and C_F are dimensionless empirical constants.^{1,2,8–10}

- The term $\varepsilon_i^{(\tau)} = \varepsilon_{iz}^{(\tau)} - \beta F_i - Q_{iz}$ in Eq. (4) is the effective dissipation rate of the off diagonal components of the Reynolds stress τ_{iz} , where $\varepsilon_{iz}^{(\tau)} = 2\nu \langle (\nabla_j u_i)^2 \rangle$ is the molecular-viscosity dissipation rate of τ_{iz} , which is small because the smallest eddies associated with viscous dissipation are presumably isotropic.⁵¹ In the framework of EFB theory, the role of the dissipation of τ_{iz} is assumed to be played by the combination of terms $-\beta F_i - Q_{iz}$, and it is assumed that $\varepsilon_i^{(\tau)} = \tau_{iz}/(C_\tau t_T)$, where C_τ is the effective-dissipation time-scale empirical constant.^{25,29}
- We assume that the term $\rho_0^{-1} \langle \theta \nabla_z p \rangle$ in Eq. (3) for the vertical turbulent flux of potential temperature is parameterized by $\tilde{C}_\theta \beta \langle \theta^2 \rangle$ with $\tilde{C}_\theta < 1$, where \tilde{C}_θ is the dimensionless empirical constant. This implies that $\beta \langle \theta^2 \rangle - \rho_0^{-1} \langle \theta \nabla_z p \rangle = C_\theta \beta \langle \theta^2 \rangle$ with the positive dimensionless empirical constant $C_\theta = 1 - \tilde{C}_\theta$, which is less than 1. We also take into account that $\langle \theta \nabla_i p \rangle$ vanishes, where $i = x, y$. The justification of these assumptions have been discussed in different contexts.^{25,29}

Note that the Kolmogorov hypothesis related to the dissipation rates of the second moments in stably stratified turbulence implies that the normalized dissipation time scale of TPE, $t_\theta/t_T \equiv C_p$, turbulent heat flux, $t_F/t_T \equiv C_F$, the components E_x of TKE, t_{zx}/t_T , and off diagonal τ_{iz} components of the Reynolds stress, $\tau_{iz}/t_T \equiv C_\tau$, is empirical constants. These dissipation time scales are normalized by the dissipation timescale of TKE. Generally, these ratios of the dissipation time scales can be functions of the gradient Richardson number. For instance, recent direct numerical simulations^{52,53} of a shear produced stably stratified turbulence in Couette flow performed for the gradient Richardson number $Ri \leq 0.17$ have shown that these ratios of the dissipation time scales are weakly decreasing functions of the gradient Richardson number. In these DNS, the Reynolds numbers based on the turbulent velocities and integral time scales are not larger than 10^3 , while in atmospheric turbulence, the Reynolds numbers are about 10^6 – 10^7 . In addition, the size of the inertial subrange of scales where the Kolmogorov spectrum for the turbulent kinetic energy has been observed in these simulations is only one decade. Since for the gradient Richardson number larger than 0.17, there are no available information about these ratios of the dissipation time scales, and we do not take into account these effects in the present study. The term $\rho_0^{-1} \langle \theta \nabla_z p \rangle$ in Eq. (3) can also contribute to the classical gradient term, $\propto E_z \nabla_z \bar{\theta}$, in the vertical turbulent flux of potential temperature.⁵² However, here we neglect this effect as well.

The EFB turbulence closure implies that turbulence is maintained by the velocity shear at any stratification.^{25,29} Indeed, the buoyancy flux, βF_z , appears in Eqs. (1) and (5) with opposite signs and describes the energy exchange between the densities of the turbulent kinetic energy and turbulent potential energy. Since in the budget equations (1) and (5), the buoyancy fluxes, $\pm \beta F_z$, enter with opposite signs, and they cancel each other in budget equation (6) for the total turbulent energy density. Therefore, as follows from Eq. (6), the density of the total turbulent energy is independent of the buoyancy. This implies that there are no grounds to consider the buoyancy-flux term in Eq. (1) for the turbulent kinetic energy density as an ultimate “killer” of turbulence. When the rates of the production and dissipation of the density of the total turbulent energy are compensated, the total turbulent energy is conserved. This implies that an increase in the vertical gradient of the mean potential temperature increases the buoyancy and decreases the density of turbulent kinetic energy, but it increases

the turbulent potential energy density so that the total turbulent energy is conserved.

The main mechanism for the self-regulation of stably stratified turbulence is as follows.^{25,29} In a steady-state and homogeneous regime of turbulence, budget equation (5) for the vertical turbulent flux F_z of the potential temperature yields

$$F_z = -C_F t_T \langle u_z^2 \rangle \nabla_z \bar{\theta} + 2 C_\theta C_F t_T \beta E_\theta. \quad (8)$$

Equation (8) implies that an increase in the vertical gradient of the mean potential temperature increases the turbulent potential energy E_p (and it increases E_θ), but it also decreases the vertical flux of potential temperature. This is because two contributions to the vertical turbulent flux F_z (the classical gradient contribution, $-C_F t_T \langle u_z^2 \rangle \nabla_z \bar{\theta}$, and the non-gradient contribution, $2 C_\theta C_F t_T \beta E_\theta$) have opposite signs. Therefore, this feedback closes a loop, i.e., this effect decreases the buoyancy and maintains stably stratified turbulence for any gradient Richardson numbers.

Thus, the correct mechanism of self-existence of a stably stratified turbulence includes two steps: (i) the conversion of turbulent kinetic energy into turbulent potential energy with the increasing vertical gradient of the mean potential temperature and (ii) self-control feedback of the negative, down-gradient turbulent heat transfer through the efficient generation of the counteracting, positive, non-gradient heat transfer by the turbulent potential energy. Due to this feedback, stably stratified turbulence is maintained up to strongly supercritical stratifications. This explains the absence of critical gradient Richardson numbers as a threshold for the existence of stably stratified turbulence.^{25,29} Actually the critical Richardson number, treated many years as a threshold between the turbulent and laminar regimes, separates two turbulent regimes: the strong turbulence typical of atmospheric boundary layers and the weak three-dimensional turbulence typical of the free atmosphere or deep ocean and characterized by a strong decrease in the heat transfer in comparison to the momentum transfer.

To quantify stably stratified turbulence, the following basic dimensionless parameters are used:

- the gradient Richardson number:

$$Ri = \frac{N^2}{S^2}, \quad (9)$$

- the flux Richardson number:

$$Ri_f = \frac{-\beta F_z}{K_M S^2}, \quad (10)$$

- the turbulent Prandtl number:

$$Pr_T = \frac{K_M}{K_H}, \quad (11)$$

where K_M is the turbulent viscosity, K_H is the turbulent diffusivity, and $S^2 = (\nabla_z \bar{U}_x)^2 + (\nabla_z \bar{U}_y)^2$ is the squared mean velocity shear.

In the framework of the EFB turbulence closure theory,^{25,29} we use assumptions outlined at the beginning of Sec. II B for the budget equations (1)–(5) for the density of TKE E_K , the intensity of potential temperature fluctuations E_θ , the vertical turbulent flux F_z of potential temperature, the horizontal turbulent flux F_i of potential temperature,

the off diagonal components of the Reynolds stress τ_{iz} , and the vertical density of TKE E_z ,

$$0 = -\tau_{iz} \nabla_z \bar{U}_i + \beta F_z - \frac{E_K}{t_T}, \tag{12}$$

$$0 = -F_z \nabla_z \bar{\Theta} - \frac{E_\theta}{C_p t_T}, \tag{13}$$

$$0 = -2E_z \nabla_z \bar{\Theta} + 2C_\theta \beta E_\theta - \frac{F_z}{C_F t_T}, \tag{14}$$

$$0 = -F_z \nabla_z \bar{U}_i - \frac{F_i}{C_F t_T}, \quad i = x, y, \tag{15}$$

$$0 = -2E_z \nabla_z \bar{U}_i - \frac{\tau_{iz}}{C_\tau t_T}, \quad i = x, y, \tag{16}$$

$$0 = \beta F_z + \frac{1}{2} Q_{zz} - \frac{E_K}{3t_T}. \tag{17}$$

Equation (16) yields expressions for the turbulent fluxes τ_{iz} of the momentum and the turbulent viscosity K_M ,

$$\tau_{iz} = -K_M \nabla_z \bar{U}_i, \quad i = x, y, \tag{18}$$

$$K_M = 2C_\tau t_T E_z. \tag{19}$$

Equation (14) allows us to obtain the expression for the vertical turbulent flux of potential temperature $F_z = -2C_F t_T (E_z - C_\theta E_p) \nabla_z \bar{\Theta}$, where we take into account that $E_\theta = E_p N^2 / \beta^2$ and $N^2 = \beta \nabla_z \bar{\Theta}$. In particular, the expression for the vertical turbulent flux F_z can be rewritten as

$$F_z = -K_H \nabla_z \bar{\Theta}, \tag{20}$$

where the coefficient of the turbulent diffusion K_H reads

$$K_H = 2C_F t_T E_z \left(1 - C_\theta \frac{E_p}{E_z} \right). \tag{21}$$

By means of Eq. (15), we find the horizontal turbulent flux F_i of potential temperature,

$$F_i = -C_F t_T F_z \nabla_z \bar{U}_i, \quad i = x, y. \tag{22}$$

Since in stably stratified turbulence, the vertical turbulent flux F_z is negative, and the horizontal turbulent flux F_i of the potential temperature is directed along the wind velocity \bar{U}_i , i.e., Eq. (22) describes the co-wind horizontal turbulent flux.

In the following, we derive expressions for useful dimensionless parameters as universal functions of the flux Richardson number. In particular, the obtained expressions for the turbulent viscosity K_M and the turbulent diffusivity K_H allow us to determine the turbulent Prandtl number $Pr_T = K_M / K_H$ as

$$Pr_T = Pr_T^{(0)} \left(1 - C_\theta \frac{E_p}{E_z} \right)^{-1}, \tag{23}$$

where $Pr_T^{(0)} = C_\tau / C_F$ is the turbulent Prandtl number at $Ri = Ri_f = 0$, i.e., for a non-stratified turbulence. Equations (10) and (12) yield the expression for the density of TKE, $E_K = K_M S^2 t_T (1 - Ri_f)$, while Eq. (13) allows us to find the intensity of potential temperature fluctuations $E_\theta = -C_p t_T F_z \nabla_z \bar{\Theta}$. This equation can be rewritten in terms

of the density of turbulent potential energy (TPE) $E_p = -\beta F_z C_p t_T$ so that the ratio E_K / E_p reads

$$\frac{E_K}{E_p} = \frac{1 - Ri_f}{C_p Ri_f}. \tag{24}$$

By means of Eq. (24), we also obtain the densities of TKE and TPE normalized by the density of the total turbulent energy (TTE), $E_T = E_K + E_p$,

$$\frac{E_K}{E_T} = \frac{1 - Ri_f}{1 - (1 - C_p) Ri_f}, \tag{25}$$

$$\frac{E_p}{E_T} = \frac{C_p Ri_f}{1 - (1 - C_p) Ri_f}. \tag{26}$$

Equations (12) and (19) allow us to obtain the dimensionless ratio

$$\left(\frac{\tau}{E_K} \right)^2 = \frac{2C_\tau A_z}{1 - Ri_f}, \tag{27}$$

where $A_z \equiv E_z / E_K$ is the vertical share of TKE, $\tau = (\tau_{xz}^2 + \tau_{yz}^2)^{1/2} = K_M S$, and $\tau_{ij} = \langle u_i u_j \rangle$ is the Reynolds stress. By means of Eqs. (19) and (27), we find the expression for another useful dimensionless parameter

$$(St_T)^2 = \frac{1}{2C_\tau A_z (1 - Ri_f)}. \tag{28}$$

In addition, Eqs. (19) and (28) allow us to obtain the dimensionless ratio

$$\frac{\beta F_z t_T}{E_K} = -\frac{Ri_f}{1 - Ri_f}, \tag{29}$$

while Eqs. (13) and (20) yield the dimensionless ratio

$$\frac{F_z^2}{E_K E_\theta} = \frac{2C_\tau A_z}{C_p Pr_T}. \tag{30}$$

Finally, applying Eqs. (23) and (24), we arrive at the useful expression for the turbulent Prandtl number Pr_T ,

$$Pr_T(Ri_f) = Pr_T^{(0)} \left(1 - \frac{C_\theta C_p Ri_f}{(1 - Ri_f) A_z} \right)^{-1}. \tag{31}$$

Since the turbulent Prandtl number can be rewritten as $Pr_T \equiv Ri / Ri_f$, Eq. (31) yields the important expression that relates the gradient Richardson number Ri and the flux Richardson number Ri_f ,

$$Ri(Ri_f) = Pr_T^{(0)} Ri_f \left(1 - \frac{C_\theta C_p Ri_f}{(1 - Ri_f) A_z} \right)^{-1}. \tag{32}$$

Expressions (27)–(28) and (30)–(32) contain the vertical share of TKE, $A_z \equiv E_z / E_K$, that will be determined below.

In shear-produced turbulence, the mean wind shear generates the energy of longitudinal velocity fluctuations E_x , which in turn feeds the transverse E_y and the vertical E_z components of the turbulent kinetic energy. The inter-component energy exchange term Q_{zx} in Eq. (5) is traditionally parameterized through the “return-to-isotropy” hypothesis (see below).⁵⁴ However, stratified turbulence is usually anisotropic, and the inter-component energy exchange term Q_{zx}

should depend on the flux Richardson number Ri_f . We adopt another model for the inter-component energy exchange term Q_{xz} , which generalizes the return-to-isotropy hypothesis to the case of stably stratified turbulence. In this model, we use the normalized flux Richardson number Ri_f/R_∞ varying from 0 for a non-stratified turbulence to 1 for a strongly stratified turbulence, where the limiting value of the flux Richardson number, $R_\infty \equiv Ri_f|_{Ri \rightarrow \infty}$, is defined for very strong stratifications when the gradient Richardson number $Ri \rightarrow \infty$. This model for the inter-component energy exchange term Q_{xz} is described by

$$Q_{xx} = -\frac{2(1 + C_r)}{3t_T} (3E_x - E_{int}), \tag{33}$$

$$Q_{yy} = -\frac{2(1 + C_r)}{3t_T} (3E_y - E_{int}), \tag{34}$$

$$Q_{zz} = -\frac{2(1 + C_r)}{3t_T} (3E_z - 3E_K + 2E_{int}), \tag{35}$$

where

$$E_{int} = E_K + \frac{Ri_f}{R_\infty} \left(\frac{C_r}{1 + C_r} \right) [C_0 E_K - (1 + C_0) E_z], \tag{36}$$

C_0 and C_r are the dimensionless empirical constants. When $Ri_f = 0$, Eqs. (33)–(36) describe the return-to-isotropy hypothesis.⁵⁴ Thus, by means of Eqs. (17), (29), (35), and (36), we determine the vertical share of TKE $A_z \equiv E_z/E_K$ as a function of the flux Richardson number Ri_f ,

$$A_z(Ri_f) = \frac{C_r (1 - 2C_0 Ri_f/R_\infty) - 3 (Ri_f^{-1} - 1)^{-1}}{3 + C_r [3 - 2(1 + C_0) Ri_f/R_\infty]}. \tag{37}$$

According to Eq. (37), the vertical share A_z of TKE varies between $(A_z)_{Ri \rightarrow 0} \equiv A_z^{(0)} = C_r/3(1 + C_r)$ for a non-stratified turbulence and $(A_z)_{Ri \rightarrow \infty} \equiv A_z^{(\infty)}$ for a strongly stratified turbulence, where

$$A_z^{(\infty)} = \frac{C_r(1 - 2C_0) - 3 (R_\infty^{-1} - 1)^{-1}}{3 + C_r(1 - 2C_0)}. \tag{38}$$

When there is an isotropy in the horizontal plane, the shares of TKE $A_x \equiv E_x/E_K$ and $A_y \equiv E_y/E_K$ in horizontal directions are given by

$$A_x = A_y = \frac{1}{2} (1 - A_z). \tag{39}$$

Now, we derive the expression for the ratio of the vertical turbulent dissipation length scale $\ell_z = t_T E_z^{1/2}$ and the local Obukhov length scale L defined as⁵⁵

$$L = \frac{\tau^{3/2}}{-\beta F_z}. \tag{40}$$

To this end, we use Eqs. (10) and (40), which yield

$$K_M = Ri_f \tau^{1/2} L. \tag{41}$$

By means of Eqs. (19), (27), and (41), we obtain the ratio ℓ_z/L as the function of the flux Richardson number,

$$\frac{\ell_z}{L} = (2 C_\tau)^{-3/4} \frac{A_z^{-1/4} Ri_f}{(1 - Ri_f)^{1/4}}. \tag{42}$$

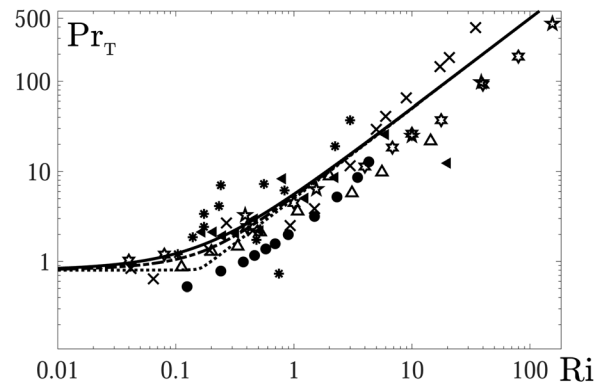


FIG. 1. The turbulent Prandtl number Pr_T vs the gradient Richardson number Ri for $A_z^{(\infty)} = 10^{-3}$ (dotted line), 0.1 (dashed-dotted line), and 0.2 (solid line). Comparison with data of meteorological observations: slanting black triangles⁵⁶ and snowflakes;⁵⁷ laboratory experiments: slanting crosses,⁵⁸ six-pointed stars,¹⁵ and black circles;¹⁴ DNS: five-pointed stars;²⁰ and LES: triangles.²⁵

For illustration, in Figs. 1–4, we show the dependencies of the following parameters on the gradient Richardson number Ri for different values of parameter $A_z^{(\infty)}$:

- the turbulent Prandtl number $Pr_T(Ri)$ given by Eq. (31) (see Fig. 1),
- the flux Richardson number $Ri_f(Ri)$ given by Eq. (32) (see Fig. 2),
- the vertical share of TKE $A_z(Ri) \equiv E_z/E_K$ given by Eq. (37) (see Fig. 3), and
- the ratio ℓ_z/L given by Eq. (42) (see Fig. 4).

The theoretical Ri -dependencies are compared with the data of meteorological observations, laboratory experiments, DNS, and LES. Figures 1–3 demonstrate reasonable agreement between theoretical predictions based on the EFB turbulence theory and data obtained from atmospheric and laboratory experiments, LES, and DNS.

Data for $Pr_T(Ri)$ at a small gradient Richardson number Ri in Fig. 1 are consistent with the commonly accepted empirical estimate of $Pr_T^{(0)} = 0.8$.^{63–65} The flux Richardson number Ri_f in the

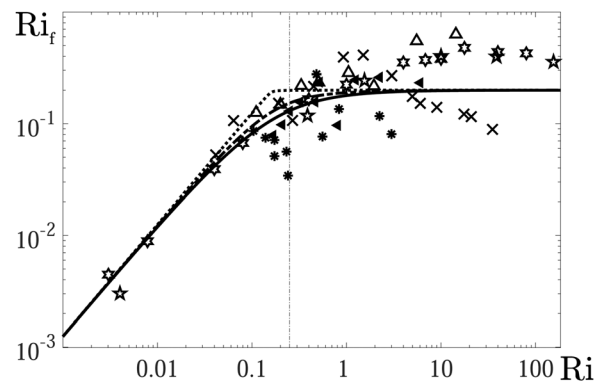


FIG. 2. The flux Richardson number Ri_f vs the gradient Richardson number Ri for $A_z^{(\infty)} = 10^{-3}$ (dotted line), 0.1 (dashed-dotted line), and 0.2 (solid line). Comparison with data of meteorological observations: slanting black triangles⁵⁶ and snowflakes;⁵⁷ laboratory experiments: slanting crosses,⁵⁸ six-pointed stars,¹⁵ and black circles;¹⁴ DNS: five-pointed stars;²⁰ and LES: triangles.²⁹

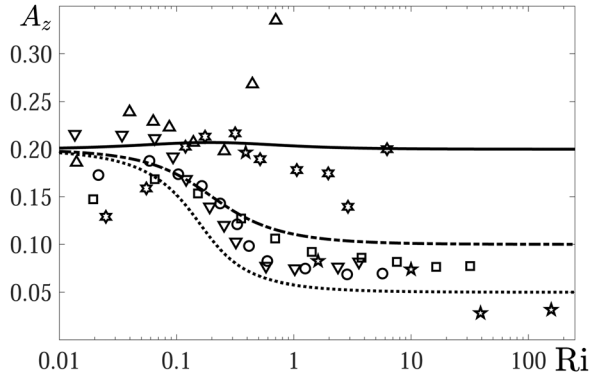


FIG. 3. The vertical share of TKE $A_z \equiv E_z/E_K$ vs the gradient Richardson number Ri for $A_z^{(\infty)} = 0.05$ (dotted line), 0.1 (dashed-dotted line), and 0.2 (solid line). Comparison with data of meteorological observations: squares,⁵⁹ circles,⁶⁰ overturned triangles,^{16,61} and six-pointed stars,⁶² laboratory experiments: six-pointed stars;¹⁵ and DNS: five-pointed stars.²⁰

steady-state regime can only increase with the increasing Ri , but obviously cannot exceed unity. Hence, it should tend to a finite asymptotic limit (estimated as $R_\infty = 0.2$), which corresponds to the asymptotically linear Ri -dependence of Pr_T . Thus, the turbulent Prandtl number for strong stratifications is given by

$$Pr_T = Pr_T^{(0)} + \frac{Ri}{R_\infty}. \quad (43)$$

Figure 2 shows that the flux Richardson number Ri_f at the gradient Richardson number $Ri > 1$ levels off at the limiting value, $Ri_f = R_\infty = 0.2$. Figures 3 and 4 demonstrate that the vertical share of TKE A_z and the ratio ℓ_z/L level off at $Ri > 1$ as well.

Let us discuss the choice of the dimensionless empirical constants.²⁹ There are two well-known universal constants: the limiting value of the flux Richardson number $R_\infty = 0.2$ for extremely strongly stratified turbulence (i.e., for $Ri \rightarrow \infty$) and the turbulent Prandtl number $Pr_T^{(0)} = 0.8$ for nonstratified turbulence (i.e., for $Ri \rightarrow 0$). The constants $C_F = C_\tau/Pr_T^{(0)}$, where C_τ is the coefficient determining the turbulent viscosity ($K_M = 2C_\tau A_z E_K^{1/2} \ell_0$) for non-stratified turbulence.

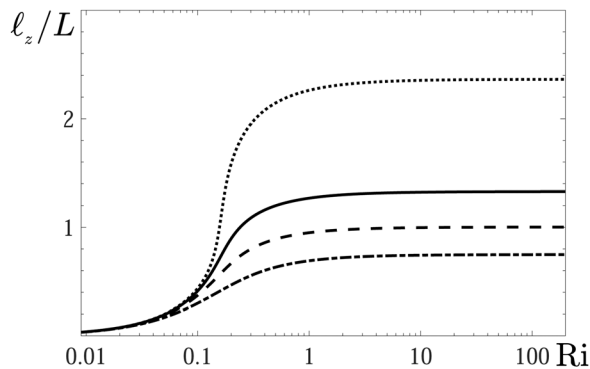


FIG. 4. The normalized vertical turbulent dissipation length scales ℓ_z/L vs the gradient Richardson number Ri for $A_z^{(\infty)} = 10^{-3}$ (dotted line), 3.1×10^{-3} (dashed line), 10^{-2} (solid line), and 0.1 (dashed-dotted line).

The constant C_p describes the deviation of the dissipation timescale of $E_\theta = \langle \theta^2 \rangle / 2$ from the dissipation timescale of TKE. The constants C_F , C_p , and $A_z^{(\infty)}$ are determined from numerous meteorological observations, laboratory experiments, direct numerical simulations (DNS), and large eddy simulations (LES).^{14,15,20,25,29,39,56–59,61,68–71} The constant C_θ is given by $C_\theta = (R_\infty^{-1} - 1) A_z^{(\infty)} / C_p$ [see Eq. (31)], and the constant C_0 is determined from Eq. (38) at given $A_z^{(\infty)}$ and C_r . We use here the following values of the non-dimensional empirical constants: $C_F = 0.125$, $C_p = 0.417$, $C_r = 3/2$, and $C_\tau = 0.1$. The vertical anisotropy parameter for extremely strongly stratified turbulence $A_z^{(\infty)}$ is mainly changing in the interval from 0.1 to 0.2 (see Fig. 3).

C. Boundary-layer turbulence

Considering the applications of the obtained results to atmospheric stably stratified boundary-layer turbulence, we derive below the theoretical relationships potentially useful in modeling applications. There are two well-known results for the wind shear:

- $S = \tau^{1/2} / \kappa z$ at $\zeta \ll 1$, which yields the log-profile for the mean velocity, and
- $S = \tau^{1/2} / R_\infty L$ when $\zeta \gg 1$, following Eq. (41). Here, $\zeta = \int_0^\zeta dz' / L(z')$ is the dimensionless height based on the local Obukhov length scale $L(z) = \tau^{3/2}(z) / [-\beta F_z(z)]$, and $\kappa = 0.4$ is the von Karman constant.

The straightforward interpolation between these two asymptotic results for the wind shear,

$$S(\zeta) = \frac{\tau^{1/2}}{L} \left(R_\infty^{-1} + \frac{1}{\kappa \zeta} \right), \quad (44)$$

yields the vertical profile of the eddy viscosity $K_M = \tau / S$ as

$$K_M(\zeta) = \tau^{1/2} L \frac{\kappa \zeta}{1 + R_\infty^{-1} \kappa \zeta}. \quad (45)$$

The vertical profile of the flux Richardson number $Ri_f(z)$ is obtained using Eqs. (41) and (45):

$$Ri_f(\zeta) = \frac{\kappa \zeta}{1 + R_\infty^{-1} \kappa \zeta}. \quad (46)$$

Now, we determine the vertical profiles of the turbulent Prandtl number $Pr_T(z)$ using Eqs. (31) and (46):

$$Pr_T(\zeta) = Pr_T^{(0)} \left[1 + \frac{a_1 \zeta + a_2 \zeta^2}{1 + a_3 \zeta} \right], \quad (47)$$

and the vertical share of TKE $A_z \equiv E_z/E_K$ by means of Eqs. (37) and (46):

$$A_z(\zeta) = \frac{C_r R_\infty + \kappa \zeta \left[C_r (1 - 2C_0) - 3(R_\infty + \kappa \zeta) [1 + \kappa \zeta (R_\infty^{-1} - 1)]^{-1} \right]}{3R_\infty (1 + C_r) + \kappa \zeta [3 + C_r (1 - 2C_0)]}. \quad (48)$$

Here, $Pr_T^{(0)} = C_\tau / C_F$, and the coefficients a_k are related to the empirical dimensionless constants:

$$a_1 = 3 \kappa A_z^{(\infty)} (1 + C_r^{-1}) (R_\infty^{-1} - 1), \quad (49)$$

$$a_2 = \frac{\kappa^2 A_z^{(\infty)}}{R_\infty} (R_\infty^{-1} - 1) (1 - 2C_0 + 3C_r^{-1}), \quad (50)$$

$$a_3 = \kappa [2R_\infty^{-1} (1 - C_0) - 3C_r^{-1} - 1] - a_1. \quad (51)$$

Next, we find the vertical profile of the gradient Richardson number applying Eqs. (32) and (46):

$$Ri(\zeta) = \frac{\kappa \zeta Pr_T^{(0)}}{1 + R_\infty^{-1} \kappa \zeta} \left[1 + \frac{a_1 \zeta + a_2 \zeta^2}{1 + a_3 \zeta} \right]. \quad (52)$$

Finally, the vertical profile of the turbulent dissipation length scale $\ell_z(z)$ normalized by the local Obukhov length scale $L(z)$ is obtained by means of Eqs. (42) and (46):

$$\frac{\ell_z}{L} = (2C_\tau)^{-3/4} \frac{A_z^{-1/4} \kappa \zeta (1 - Ri_f/R_\infty)}{(1 - Ri_f)^{1/4}}. \quad (53)$$

Equations (45)–(53) for the surface layer ($\zeta \ll 1$) have been derived in Refs. 28 and 29. In the present study, we generalize these results for the entire stably stratified boundary layer that are valid for arbitrary values of ζ .

Equations (45)–(53) are in agreement with the Monin–Obukhov⁶⁶ and Nieuwstadt⁶⁷ similarity theories, i.e., the concept of similarity of turbulence in terms of the dimensionless height $\zeta = \int_0^z dz'/L(z')$. The Monin–Obukhov similarity theory was designed for the “surface layer” defined as the lower layer that is 10% of the boundary layer, where the turbulent fluxes of momentum τ , heat F_z , and other scalars, as well as the length scale L , are approximated by their surface values. Nieuwstadt⁶⁷ extended the similarity theory to the entire stably stratified boundary layer employing local z -dependent values of the turbulent fluxes $\tau(z)$ and $F_z(z)$ and the length $L(z)$ instead of their surface values.

For illustration, in Figs. 5–9, we plot the vertical profiles of the key turbulent parameters:

- the gradient Richardson number $Ri(\zeta)$ given by Eq. (52) (see Fig. 5),
- the flux Richardson number $Ri_f(\zeta)$ given by Eq. (46) (see Fig. 6),

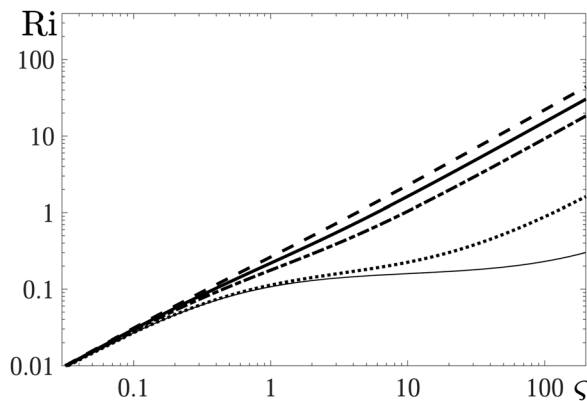


FIG. 5. The gradient Richardson number Ri vs $\zeta = \int_0^z dz'/L(z')$ for $A_z^{(\infty)} = 10^{-3}$ (solid thin line), 10^{-2} (dotted line), 0.1 (dashed-dotted line), 0.15 (solid thick line), and 0.2 (dashed line).

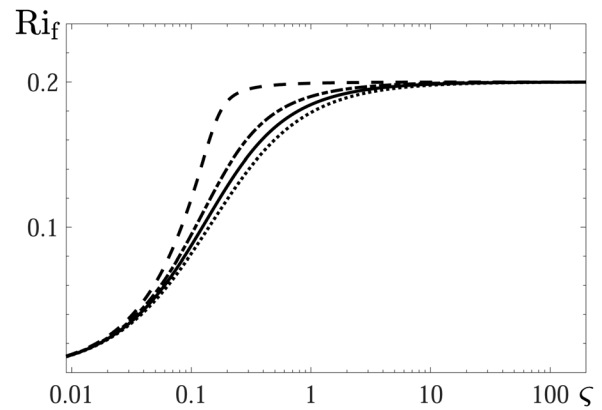


FIG. 6. The flux Richardson number Ri_f vs $\zeta = \int_0^z dz'/L(z')$ for $A_z^{(\infty)} = 10^{-2}$ (dashed line), 0.1 (dashed-dotted line), 0.15 (solid line), and 0.2 (dotted line).

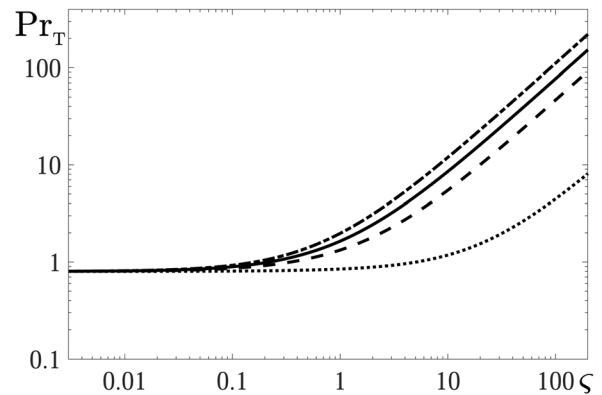


FIG. 7. The turbulent Prandtl number Pr_T vs $\zeta = \int_0^z dz'/L(z')$ for $A_z^{(\infty)} = 10^{-2}$ (dotted line), 0.1 (dashed line), 0.15 (solid line), and 0.2 (dashed-dotted line).

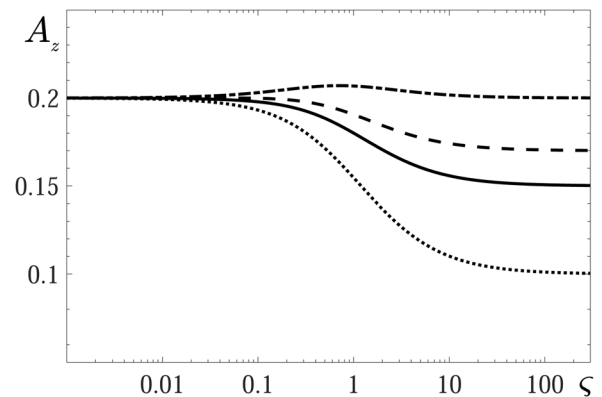


FIG. 8. The vertical share of TKE $A_z \equiv E_z/E_\kappa$ vs $\zeta = \int_0^z dz'/L(z')$ for different $A_z^{(\infty)} = 0.1$ (dotted line), 0.15 (solid line), 0.17 (dashed line), and 0.2 (dashed-dotted line).

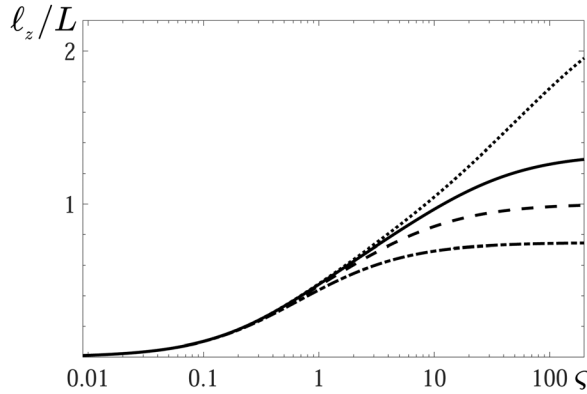


FIG. 9. The normalized vertical turbulent dissipation length scales ℓ_z/L vs $\zeta = \int_0^z dz'/L(z')$ for different $A_z^{(\infty)} = 0.1$ (dotted line), 0.15 (solid line), 0.17 (dashed line), and 0.2 (dashed-dotted line).

- the turbulent Prandtl number $Pr_T(\zeta)$ given by Eq. (47) (see Fig. 7),
- the vertical share of TKE $A_z(\zeta) \equiv E_z/E_K$ given by Eq. (48) (see Fig. 8), and
- the normalized vertical turbulent dissipation length scales ℓ_z/L vs ζ given by Eq. (53) (see Fig. 9).

Different lines in Figs. 5–9 correspond to different values of $A_z^{(\infty)}$ (see below). As follows from Fig. 5 for the vertical profile of $Ri(z)$, the gradient Richardson number increases with height, and the case $\zeta < 1$ corresponds to $Ri < 0.3$, while $Ri > 1$ when $\zeta > 10$. Similarly, Fig. 6 for the vertical profile of $Ri_f(z)$ shows that the flux Richardson number increases with height and levels off at $\zeta > 10$. The turbulent Prandtl number Pr_T is constant at $\zeta < 0.1$ and linearly increases at $\zeta > 2$ for $A_z^{(\infty)} \geq 0.1$ (and at $\zeta > 20$ for $A_z^{(\infty)} \ll 0.1$) (see Fig. 7). The vertical share of TKE A_z decreases with the increasing height (in all cases except one shown by the dashed-dotted line, see below), and at $\zeta > 100$, it levels off (see Fig. 8). It is clear that stable stratification, suppressing the vertical component E_z of TKE, facilitates the energy exchange between the horizontal velocity energies E_x and E_y and, thereby, causes a tendency toward isotropy in the horizontal plane. Equation (52) for the vertical turbulent dissipation length scale ℓ_z has quite expected asymptotes: $\ell_z \propto z$ at $\zeta \ll 1$ and $\ell_z \propto L$ when $\zeta > 1$ (see Fig. 9), where $\zeta = \int_0^z dz'/L(z')$. In Secs. III A–III C, we develop the energy and flux budget turbulence closure theory for passive scalars.

III THE EFB THEORY FOR PASSIVE SCALARS

In this section, we discuss energy and flux budget turbulence closure theory for passive scalars.

A. Budget equation for the turbulent flux of particles

We consider passive (non-buoyant, non-inertial) particles suspended in the turbulent fluid flow with large Reynolds numbers. The evolution of the particle number density $n_p(t, \mathbf{r})$ (measured in m^{-3}) is determined by the following equation:

$$\frac{\partial n_p}{\partial t} + (\mathbf{v} \cdot \nabla)n_p = \chi \Delta n_p, \quad (54)$$

where \mathbf{v} is an incompressible fluid velocity field and χ is the coefficient of molecular (Brownian) diffusion. Particle number density $n_p = \bar{n} + n$ is characterized by the mean value \bar{n} and fluctuations n . Averaging this equation over ensemble of velocity fluctuations, we obtain the equation for the mean particle number density \bar{n} . Subtracting this equation from Eq. (54), we obtain the equation for particle number density fluctuations as

$$\frac{Dn}{Dt} = -(\mathbf{u} \cdot \nabla)\bar{n} - (\mathbf{u} \cdot \nabla)n + \langle (\mathbf{u} \cdot \nabla)n \rangle + \chi \Delta n. \quad (55)$$

For non-inertial particles, the main effect of turbulent transport is the turbulent diffusion, i.e., the turbulent particle flux is $F_i^{(n)} \equiv \langle u_i n \rangle = -K_{ij} \nabla_j \bar{n}$. This implies that the quadratic form $K_{ij} (\nabla_i \bar{n}) (\nabla_j \bar{n})$ should be positively defined. This means that $\partial \bar{n}^2 / \partial t < 0$, i.e., the tensor K_{ij} is indeed describes a dissipative process.

Multiplying Eq. (55) by u_i and the Navier–Stokes equation by n , taking the sum and averaging the obtained equation over an ensemble, we obtain the budget equation for the turbulent flux of particles $F_i^{(n)} = \langle u_i n \rangle$,

$$\frac{DF_i^{(n)}}{Dt} + \nabla_z \tilde{\Phi}_i^{(n)} = -\langle u_i u_j \rangle \nabla_j \bar{n} - F_j^{(n)} \nabla_j \bar{U}_i + Q_i^{(n)} - \varepsilon_i^{(n)}, \quad (56)$$

where $\tilde{\Phi}_i^{(n)} = \langle u_i u_z n \rangle + \rho_0^{-1} \langle p n \rangle \delta_{i3} - \chi \langle u_i \nabla_z n \rangle - \nu \langle n \nabla_z u_i \rangle$ is the third-order moment that determines the turbulent flux of $F_i^{(n)}$, while $\varepsilon_i^{(n)} = (\nu + \chi) \langle (\nabla_j u_i) (\nabla_j n) \rangle$ is the molecular dissipation rate of $F_i^{(n)}$. The Kolmogorov closure hypothesis implies that $\varepsilon_i^{(n)} = F_i^{(n)} / C_n t_T$, where C_n is an empirical dimensionless coefficient. The term $Q_i^{(n)} = \rho_0^{-1} \langle p \nabla_i n \rangle + \beta e_i \langle n \theta \rangle$ in Eq. (56) is derived in the Appendix as

$$Q_i^{(n)} = -\frac{C_D}{2} \beta t_T e_i F_j^{(n)} \nabla_j \bar{\Theta} + \beta \nabla_i \langle n \Delta^{-1} \nabla_z \theta \rangle, \quad (57)$$

where \mathbf{e} is the vertical unit vector and C_D is an empirical dimensionless constant. Thus, the budget equation for the turbulent flux of particles can be rewritten as

$$\begin{aligned} \frac{DF_i^{(n)}}{Dt} + \nabla_z \Phi_i^{(n)} = & -\frac{C_D}{2} \beta t_T e_i F_j^{(n)} \nabla_j \bar{\Theta} - \tau_{ij} \nabla_j \bar{n} \\ & - F_j^{(n)} \nabla_j \bar{U}_i - \frac{F_i^{(n)}}{C_n t_T}, \end{aligned} \quad (58)$$

where $\Phi_i^{(n)} = \tilde{\Phi}_i^{(n)} - \beta e_i \langle n \Delta^{-1} \nabla_z \theta \rangle$. Equation (58) yields the budget equation for the vertical particle flux $F_z^{(n)}$ as

$$\frac{DF_z^{(n)}}{Dt} + \nabla_z \Phi_z^{(n)} = -2E_z \nabla_z \bar{n} - \frac{1}{2} C_D \beta t_T F_z^{(n)} \nabla_z \bar{\Theta} - \frac{F_z^{(n)}}{C_n t_T}. \quad (59)$$

In Eq. (59), we have taken into account that $|K_M S_i \nabla_i \bar{n}| \ll |2E_z \nabla_z \bar{n}|$, where $S_i \equiv S_{x,y} = \nabla_z \bar{U}_{x,y}$. We will demonstrate that this condition provides the positively defined quadratic form $K_{ij} (\nabla_i \bar{n}) (\nabla_j \bar{n})$. Equations (58) and (59) are complementary equations to the EFB turbulence closure theory discussed in Sec. II.^{25,29} These equations allow us to determine the turbulent flux of particles $F_i^{(n)}$ at a given gradient of the mean particle number density \bar{n} and the basic turbulent parameters E_K and t_T .

B. Turbulent flux of particles and turbulent diffusion tensors

In air pollution, modeling the particle number density \bar{n} could be strongly heterogeneous in all three directions. Limiting to the steady-state, the homogeneous regime of turbulence, Eq. (59) reduces to the turbulent diffusion formulation for the vertical turbulent flux of the passive scalar (i.e., non-inertial particles),

$$F_z^{(n)} = -K_{zz} \nabla_z \bar{n}, \tag{60}$$

where

$$K_{zz} = K_M \left(Sc_T^{(0)} + \frac{C_D Ri}{4 A_z (1 - Ri_f)} \right)^{-1}, \tag{61}$$

$Sc_T^{(0)} = C_\tau / C_n$ and $K_{zx} = K_{zy} = 0$. Using Eqs. (18) and (19), we determine the turbulent Schmidt number as

$$Sc_T \equiv \frac{K_M}{K_{zz}} = Sc_T^{(0)} + \frac{C_D Ri}{4 A_z (1 - Ri_f)}. \tag{62}$$

In derivation of Eq. (61), we take into account that

$$N^2 t_T^2 = \frac{Ri}{2 C_\tau A_z (1 - Ri_f)}, \tag{63}$$

which follows from the identities $Ri = Ri_f Pr_T$ and Eq. (27).

The horizontal components of the turbulent flux of particles can be determined through the steady-state version of Eq. (58) for homogeneous stably stratified turbulence,

$$F_x^{(n)} = -K_{xx} \nabla_x \bar{n} - K_{xz} \nabla_z \bar{n}, \tag{64}$$

$$F_y^{(n)} = -K_{yy} \nabla_y \bar{n} - K_{yz} \nabla_z \bar{n}, \tag{65}$$

where

$$K_{xx} = 2 C_n t_T E_x = \frac{A_x}{A_z Sc_T^{(0)}} K_M, \tag{66}$$

$$K_{yy} = 2 C_n t_T E_y = \frac{A_y}{A_z Sc_T^{(0)}} K_M, \tag{67}$$

$$K_{xz} = -C_n t_T S_x K_{zz}, \tag{68}$$

$$K_{yz} = -C_n t_T S_y K_{zz}, \tag{69}$$

where $S_{x,y} = \nabla_z \bar{U}_{x,y}$ and $K_{xy} = K_{yx} = 0$. In Eqs. (64) and (65), we have taken into account a condition that provides the positively defined quadratic form $K_{ij} (\nabla_i \bar{n}) (\nabla_j \bar{n})$. In particular, this condition implies that

$$A_x > \frac{C_n}{4 Sc_T (Ri_f)} \left[\frac{C_\tau A_z (Ri_f)}{2(1 - Ri_f)} \right]^{1/2}. \tag{70}$$

Let us discuss the physics related to the off diagonal terms of the turbulent diffusion tensor of particles. To this end, we rewrite the horizontal turbulent flux of particles $F_x^{off} \equiv -K_{xz} \nabla_z \bar{n}$ that describes the off diagonal component K_{xz} of the turbulent diffusion tensor as

$$F_x^{off} = -C_n t_T F_z^{(n)} \nabla_z \bar{U}_x, \tag{71}$$

where $F_z^{(n)} = -K_{zz} \nabla_z \bar{n}$ is the vertical turbulent flux of particles [see Eq. (60)]. The turbulent flux of particles F_x^{off} given by Eq. (71) can be compared with the horizontal turbulent flux F_x of potential

temperature $F_x = -C_F t_T F_z \nabla_z \bar{U}_x$ [see Eq. (22)]. The latter flux describes the co-wind horizontal turbulent flux of potential temperature. For simplicity, we consider here the case when the wind velocity \bar{U}_x is directed along the x axis. We remind that in stably stratified turbulence, the vertical turbulent flux F_z of potential temperature is negative so that the horizontal turbulent flux F_x of potential temperature is directed along the wind velocity \bar{U}_x .

On the contrary, in convective turbulence, the vertical turbulent flux F_z of potential temperature is positive so that the horizontal turbulent flux F_x of potential temperature is a counterwind turbulent flux. The physics of the counterwind turbulent flux is the following. Let us consider horizontally homogeneous, sheared convective turbulence. With the increasing height in convection, the mean shear velocity \bar{U}_x increases and mean potential temperature $\bar{\Theta}$ decreases. Thus, uprising fluid particles produce positive fluctuations of potential temperature, $\theta > 0$ [since $\partial\theta/\partial t \propto -(\mathbf{u} \cdot \nabla)\bar{\Theta}$], and negative fluctuations of horizontal velocity, $u_x < 0$ [since $\partial u_x/\partial t \propto -(\mathbf{u} \cdot \nabla)\bar{U}_x$]. This causes negative horizontal temperature flux: $u_x \theta < 0$. Likewise, sinking fluid particles produce negative fluctuations of potential temperature, $\theta < 0$, and positive fluctuations of horizontal velocity, $u_x > 0$, also causing negative horizontal temperature flux $u_x \theta < 0$. This implies that the net horizontal turbulent flux is negative, $\langle u_x \theta \rangle < 0$, in spite of a zero horizontal mean temperature gradient. Thus, the counterwind turbulent flux of potential temperature describes the modification of the potential-temperature flux by the non-uniform velocity field. The counterwind or co-wind turbulent fluxes are associated with non-gradient turbulence transport of heat.

The comparison of two fluxes, F_x^{off} and F_x , shows that the form of the horizontal turbulent flux of particles F_x^{off} is similar to that of the horizontal turbulent flux of potential temperature F_x . For instance, when the vertical turbulent flux of particles $F_z^{(n)}$ is positive (or negative), the horizontal turbulent flux of particles F_x^{off} describes the counterwind (or the co-wind) horizontal turbulent flux of particles. These turbulent fluxes are associated with non-gradient turbulence transport of particles.

For illustration, in Figs. 10–12, we show the dependencies of the key passive scalar parameters on the gradient Richardson number Ri :

- the turbulent Schmidt number $Sc_T(Ri)$ given by Eq. (62) (see Fig. 10),

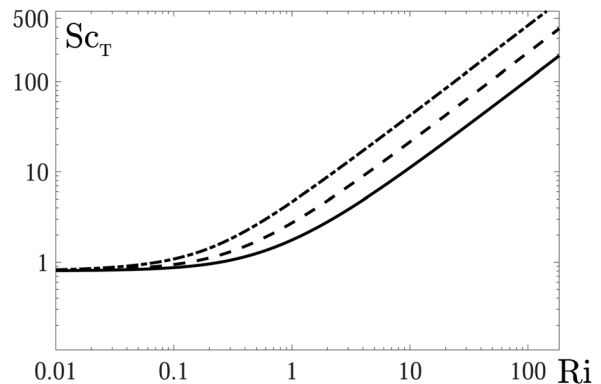


FIG. 10. The turbulent Schmidt number Sc_T vs the gradient Richardson number Ri for $A_z^{(\infty)} = 0.15$ and different values of $C_D = 0.5$ (solid line); 1 (dashed line) and 2 (dashed-dotted line).

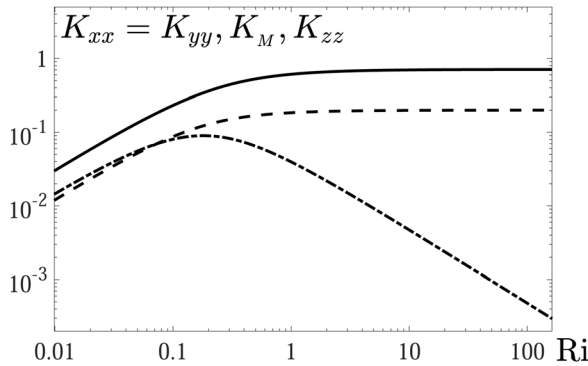


FIG. 11. Diagonal components of the turbulent diffusion tensor: $K_{xx} = K_{yy}$ (solid line) and K_{zz} (dashed-dotted line) and the eddy viscosity: K_M (dashed line) normalized by $u_* L$ vs the gradient Richardson number Ri for $A_z^{(\infty)} = 0.15$, where $C_D = 2$ and $C_n = 1$.

- the diagonal components $K_{zz}(Ri)$ and $K_{xx}(Ri) = K_{yy}(Ri)$ of the turbulent diffusion tensor normalized by $u_* L$ and given by Eqs. (61) and (66) (see Fig. 11), and
- the off diagonal component $K_{xz}(Ri)$ of the turbulent diffusion tensor normalized by $u_* L$ and given by Eq. (68) (see Fig. 12).

Here, $u_* = \tau^{1/2}$, and we consider for simplicity the cases $S_y = 0$ and $A_x = A_y$. The turbulent Schmidt number $Sc_T(Ri)$ linearly increases with the gradient Richardson number for $Ri > 1$ (see Fig. 10). As follows from Eq. (61) and Fig. 11, the vertical turbulent diffusion coefficient $K_{zz}(Ri)$ of particles or gaseous admixtures is strongly suppressed for large gradient Richardson numbers. The vertical turbulent diffusion coefficient and the turbulent Schmidt number behave in the similar fashion as the turbulent diffusion coefficient $K_H(Ri)$ of the mean potential temperature and the turbulent Prandtl number $Pr_T(Ri)$.

The physics of such a behavior of the vertical turbulent diffusion coefficient $K_{zz}(Ri)$ is related to the buoyancy force that causes a correlation between the potential temperature and the particle number density fluctuations $\langle \theta n \rangle$. This correlation is proportional to the product of the vertical turbulent particle flux $\langle n u_z \rangle$ and the vertical gradient of the mean potential temperature $\nabla_z \bar{\Theta}$, i.e., $\langle \theta n \rangle \propto -\langle n u_z \rangle \nabla_z \bar{\Theta}$.

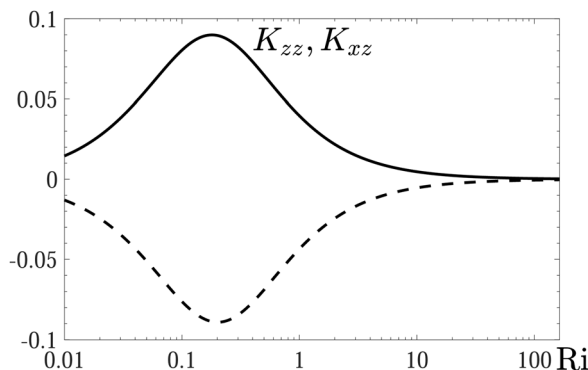


FIG. 12. Off diagonal component of the turbulent diffusion tensor: K_{xz} (dashed line) normalized by $u_* L$ vs the gradient Richardson number Ri for $A_z^{(\infty)} = 0.15$. For comparison, the diagonal component $K_{zz}(Ri)$ (solid line) is also shown here, where $C_D = 2$ and $C_n = 1$.

This correlation reduces a standard vertical turbulent particle flux $\langle n u_z \rangle$ that is proportional to the vertical gradient of the mean particle number density, $-\nabla_z \bar{n}$.

Let us consider for simplicity the case $S_y = 0$. The quadratic form $K_{ij}(\nabla_i \bar{n})(\nabla_j \bar{n})$ is positively defined if the determinant $D_{SI} = K_{xx} K_{yy} K_{zz} P_{SI}$ of the symmetric matrix \tilde{K}_{ij} is positive, where $P_{SI} = 1 - \tilde{K}_{xz}^2 / (4K_{xx} K_{zz})$ and the diagonal elements K_{xx} , K_{yy} , and K_{zz} are positive. In the symmetric matrix \tilde{K}_{ij} , the off diagonal elements $\tilde{K}_{xz} = \tilde{K}_{zx} = K_{xz}/2$ and other off diagonal elements vanish. The parameter $P_{SI}(Ri) = 1 - K_{xz}^2 / (16K_{xx} K_{zz})$ vs the gradient Richardson number is shown in Fig. 13, where we use Eqs. (61), (66), and (68). Figure 13 shows that P_{SI} and the determinant D_{SI} are always positive so that the quadratic form $K_{ij}(\nabla_i \bar{n})(\nabla_j \bar{n})$ is the positively defined quadratic form.

In view of the above analysis, the down-gradient formulation: $F_\alpha^{(n)} = -K_\alpha \nabla_\alpha \bar{n}$, where K_α are the turbulent diffusion coefficients along $\alpha = x, y, z$ axes, widely used in operational models, can hardly be considered as satisfactory. It is long ago understood that the linear dependence between the vectors $F_\alpha^{(n)}$ and $\nabla_\alpha \bar{n}$ is characterized by an eddy diffusivity tensor with non-zero off diagonal terms.⁷² Equations (61) and (66)–(69) allow determining all components of this tensor. The equations derived in this section are immediately applicable to turbulent diffusion of gaseous admixtures. In this case, \bar{n} and n denote mean value and fluctuations of the admixture concentration (measured in kg/m^3), respectively.

In temperature stratified fluids, there is an additional mechanism of particle transport, namely, turbulent thermal diffusion, which causes particle concentration in the vicinity of the mean temperature minimum, i.e., this effect results in the particle transport in the direction opposite to the temperature gradient.^{73–76} This effect has been detected in laboratory experiments,⁷⁷ DNS,⁷⁸ and atmospheric observations.⁷⁹ In the present paper, this mechanism is not considered.

C. Application to boundary-layer turbulence

Let us consider the applications of the obtained results of particle transport to the atmospheric stably stratified boundary-layer turbulence. Equations (45)–(52) allow us to find the vertical profiles of the turbulent Schmidt number and of the components of the turbulent diffusion tensor K_{ij} in the atmospheric boundary-layer turbulence. For

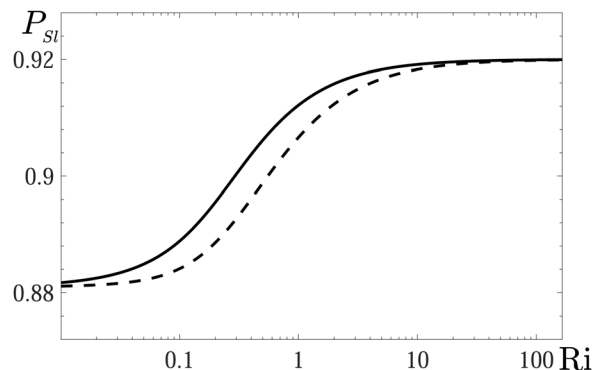


FIG. 13. The parameter $P_{SI} = 1 - K_{xz}^2 / (K_{xx} K_{zz})$ vs the gradient Richardson number Ri for $C_D = 1$ (dashed line) and 2 (dashed-dotted line) and for $A_z^{(\infty)} = 0.15$.

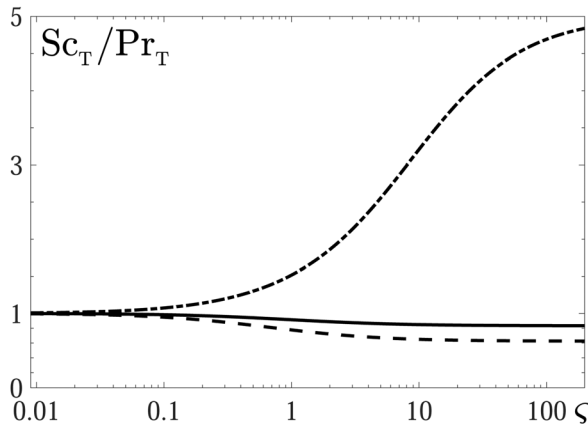


FIG. 14. The ratio Sc_T/Pr_T of the turbulent Schmidt number to turbulent Prandtl number vs $\zeta = \int_0^z dz'/L(z')$ for $C_D=2$ and different values of $A_z^{(\infty)} = 0.025$ (dashed-dotted line), 0.15 (solid line), and 0.2 (dashed line).

illustration, in Figs. 14–16 we plot the vertical profiles of the key passive scalar parameters:

- the ratio $Sc_T(\zeta)/Pr_T(\zeta)$ of the turbulent Schmidt number to turbulent Prandtl number given by Eqs. (47) and (62) (see Fig. 14),
- the diagonal components of the turbulent diffusion tensors: $K_{zz}(\zeta)$ and $K_{xx}(\zeta) = K_{yy}(\zeta)$ normalized by $u_* L$ and given by Eqs. (61) and (66) (see Fig. 15), and
- the off diagonal component of the turbulent diffusion tensor: $K_{xz}(\zeta)$ normalized by $u_* L$ and given by Eq. (68) (see Fig. 16), where we also use Eqs. (39) and (45)–(52).

Figure 14 demonstrates that the ratio Sc_T/Pr_T can be more or less than 1 depending on the parameter C_D . This implies that the turbulent Schmidt number Sc_T generally does not coincide with the turbulent Prandtl number Pr_T . This is not surprising, since temperature fluctuations cannot be considered as a passive scalar, because they strongly affect velocity fluctuations when the gradient Richardson number is not small.⁴⁶ On the other hand, fluctuations of the number

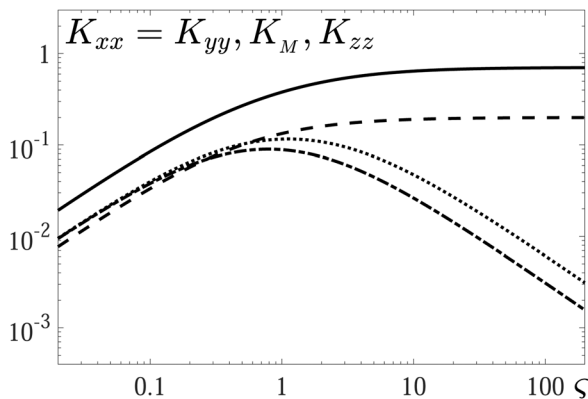


FIG. 15. Diagonal components of the turbulent diffusion tensor: $K_{xx} = K_{yy}$ (solid line) and for different values of $C_D = 1$ (dotted) and 2 (dashed-dotted), and the eddy viscosity: K_M (dashed line) normalized by $u_* L$ vs $\zeta = \int_0^z dz'/L(z')$ for $A_z^{(\infty)} = 0.15$.

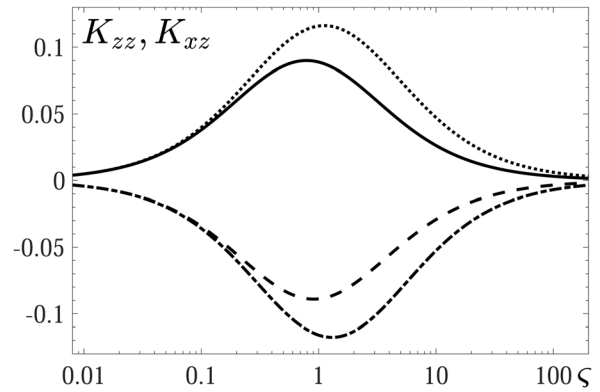


FIG. 16. Off diagonal component of the turbulent diffusion tensor: K_{xz} normalized by $u_* L$ vs $\zeta = \int_0^z dz'/L(z')$ for $C_D = 1$ (dashed line), 2 (dashed-dotted line) and for $A_z^{(\infty)} = 0.15$. For comparison, the diagonal component $K_{zz}(z/L)$ for $C_D = 1$ (dotted line) and 2 (solid line) is also shown here.

density of non-inertial particles or gaseous admixtures behave as passive scalars because they do not affect velocity fluctuations. Only fluctuations of the number density of inertial particles when the mass-loading parameter $m_p n/\rho$ is not small ($m_p n/\rho > 1$) can affect velocity fluctuations, where m_p is a particle mass.

Let us discuss the vertical profiles of the turbulent diffusion tensor K_{ij} shown in Figs. 15 and 16. Figure 15 demonstrates that the vertical turbulent diffusion coefficient K_{zz} of particles or gaseous admixtures is strongly suppressed when $\zeta \gg 10$. Equations (61) and (66)–(69) and Figs. 11, 12, 15, and 16 show that the components $K_{xx} = K_{yy}$ of the turbulent diffusion tensor in the horizontal direction are dominant in comparison with the vertical component K_{zz} . This implies that any initially created strongly inhomogeneous distribution of particles (i.e., a strong particle cluster or blob) is evolved into a thin “pancake” in the horizontal plane with a very small increase in its thickness in the vertical direction. For instance, when the vertical turbulent heat flux $|F_z| = 0.3$ K m/s, the friction velocity $u_* = 0.1$ m/s, at the height $z = 1$ km, the gradient Richardson number $Ri = 3$ (see Fig. 5), the ratio $K_{xx}/K_{zz} \approx 10^3$ (see Fig. 15) so that the horizontal size of the pancake of particles is 30 times larger than the vertical size.

IV. CONCLUSIONS

We discuss here the energy and flux budget turbulence closure theory for a passive scalar (e.g., non-buoyant and non-inertial particles or gaseous admixtures) in stably stratified turbulence. The EFB turbulence closure theory is based on the budget equations for the turbulent kinetic and potential energies and turbulent fluxes of momentum and buoyancy and the turbulent flux of particles. The EFB closure theory explains the existence of the shear produced turbulence even for very strong stratifications.

In the framework of the EFB closure theory, we have found that in a steady-state homogeneous regime of turbulence, there is a universal flux Richardson number dependence of the turbulent flux of the passive scalar described in terms of an anisotropic non-symmetric turbulent diffusion tensor. We have shown that the diagonal component in the vertical direction of the turbulent diffusion tensor for particles or gaseous admixtures is strongly suppressed for large gradient Richardson numbers, but the diagonal components in the horizontal

directions are not suppressed by strong stratification. We have determined the turbulent Schmidt number defined as the ratio of the eddy viscosity and the vertical turbulent diffusivity of the passive scalar, which linearly increases with the gradient Richardson number.

We explain these features by the effect of the buoyancy force, which causes a correlation between fluctuations of the potential temperature and the particle number density. In particular, this correlation is proportional to the product of the vertical turbulent particle flux and the vertical gradient of the mean potential temperature, which reduces the vertical turbulent particle flux.

In view of applications to atmospheric stably stratified boundary-layer turbulence, we derive the theoretical relationships for the vertical profiles of the key parameters of stably stratified turbulence measured in the units of the local Obukhov length scale. These relationships allow us to determine the vertical profiles of the components of the turbulent diffusion tensor and the turbulent Schmidt number. These results are potentially useful in modeling applications of transport of particles or gaseous admixtures in stably stratified atmospheric boundary-layer turbulence and free atmosphere turbulence.

DEDICATION

This work was dedicated to Professor Sergej Zilitinkevich (1936–2021) who initiated this work.

ACKNOWLEDGMENTS

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APPENDIX: DERIVATION OF THE BUDGET EQUATION FOR $\langle n \theta \rangle$ AND EQ. (57)

Equations for fluctuations of the potential temperature and the particle number density read as follows:

$$\frac{D\theta}{Dt} = -(\mathbf{u} \cdot \nabla)(\bar{\Theta} + \theta) + \langle (\mathbf{u} \cdot \nabla)\theta \rangle + \kappa \Delta \theta, \quad (\text{A1})$$

$$\frac{Dn}{Dt} = -(\mathbf{u} \cdot \nabla)(\bar{n} + n) + \langle (\mathbf{u} \cdot \nabla)n \rangle + \chi \Delta n. \quad (\text{A2})$$

Multiplying Eq. (A1) by n and Eq. (A2) by θ , averaging and adding the obtained equations, we arrive at the budget equation for the correlation function $\langle n \theta \rangle$,

$$\frac{D\langle n \theta \rangle}{Dt} + \nabla_j \Phi_j^{(n\theta)} = -F_j^{(n)} \nabla_j \bar{\Theta} - \varepsilon^{(n\theta)}. \quad (\text{A3})$$

Here, $\Phi_j^{(n\theta)}$ is the third-order moment describing the turbulent flux of the correlation function $\langle n \theta \rangle$:

$$\Phi_i^{(n\theta)} = \langle u_i n \theta \rangle - \chi \langle \theta \nabla_i n \rangle - \kappa \langle n \nabla_i \theta \rangle, \quad (\text{A4})$$

and $\varepsilon^{(n\theta)}$ is the dissipation rate of $\langle n \theta \rangle$. We assume here that the term $-F_j \nabla_j \bar{n}$ contributes to an effective dissipation of $\langle n \theta \rangle$, similarly to the effective dissipation of the Reynolds stress, i.e.,

$$\varepsilon^{(n\theta)} = (\kappa + \chi) \langle (\nabla_j n) (\nabla_j \theta) \rangle - F_j \nabla_j \bar{n}. \quad (\text{A5})$$

This assumption allows us to provide a positive dissipation rate of passive scalar fluctuations. The effective dissipation rate $\varepsilon^{(n\theta)}$ can be expressed using the Kolmogorov closure hypothesis:

$$\varepsilon^{(n\theta)} = \frac{\langle n \theta \rangle}{C_{n\theta} t_\Gamma}, \quad (\text{A6})$$

where $C_{n\theta}$ is the dimensionless constant. In the steady-state, homogeneous regime of turbulence, Eq. (A3) reduces to the turbulent diffusion formulation:

$$\langle n \theta \rangle = -C_{n\theta} t_\Gamma F_j^{(n)} \nabla_j \bar{\Theta}, \quad (\text{A7})$$

where we consider only gradient approximation neglecting higher spatial derivatives.

Now let us determine the term $Q_i^{(n)} = \rho_0^{-1} \langle p \nabla_i n \rangle + \beta e_i \langle n \theta \rangle$. Calculating the divergence of the Navier–Stokes, we obtain

$$\rho_0^{-1} \nabla^2 p = \beta \nabla_z \theta. \quad (\text{A8})$$

Applying the inverse Laplacian to Eq. (A8), we arrive at the following identity:

$$\rho_0^{-1} p = \beta \Delta^{-1} \nabla_z \theta, \quad (\text{A9})$$

which yields

$$\rho_0^{-1} \langle \theta \nabla_z p \rangle = \beta \langle \theta \Delta^{-1} \nabla_z^2 \theta \rangle. \quad (\text{A10})$$

Using Eqs. (A9) and (A10), we determine $\rho_0^{-1} \langle p \nabla_i n \rangle$:

$$\begin{aligned} \rho_0^{-1} \langle p \nabla_i n \rangle &= \beta \langle (\nabla_i n) \Delta^{-1} \nabla_i \theta \rangle = \beta \nabla_i \langle n \Delta^{-1} \nabla_z \theta \rangle \\ &\quad - \beta \langle n \Delta^{-1} \nabla_z \nabla_i \theta \rangle. \end{aligned} \quad (\text{A11})$$

Let us determine the correlation function $\langle n \Delta^{-1} \nabla_z^2 \theta \rangle$:

$$\begin{aligned} \langle n(t, \mathbf{x}) \Delta^{-1} \nabla_z^2 \theta(t, \mathbf{x}) \rangle &= \lim_{\mathbf{x} \rightarrow \mathbf{y}} \langle n(t, \mathbf{x}) \Delta^{-1} \nabla_z^2 \theta(t, \mathbf{y}) \rangle \\ &= \int \left(\frac{k_z^2}{k^2} \right) \langle n(\mathbf{k}) \theta(-\mathbf{k}) \rangle d\mathbf{k}. \end{aligned} \quad (\text{A12})$$

First, we consider an isotropic turbulence. The second moment, $\langle n(\mathbf{k}) \theta(-\mathbf{k}) \rangle$, of potential temperature fluctuations in a homogeneous and incompressible turbulence in a Fourier space reads as follows:

$$\langle n(\mathbf{k}) \theta(-\mathbf{k}) \rangle = \frac{\langle n \theta \rangle E_{n\theta}(k)}{4\pi k^2}, \quad (\text{A13})$$

where the spectrum function is $E_{n\theta}(k) = k_0^{-1} (2/3) (k/k_0)^{-5/3}$ for large Reynolds numbers. Here, $k_0 \leq k \leq k_D$, where the wave number $k_0 = 1/\ell_0$, with the length ℓ_0 being the integral scale and the wave number $k_D = \ell_D^{-1}$, with $\ell_D = \ell_0 \text{Pe}^{-3/4}$ being the diffusion scale and $\text{Pe} = u_0 \ell_0 / D \gg 1$ being the Péclet number. Therefore,

$$\begin{aligned} \langle n(t, \mathbf{x}) \Delta^{-1} \nabla_z^2 \theta(t, \mathbf{x}) \rangle &= \frac{\langle n \theta \rangle}{4\pi} \int_{k_0}^{\infty} E_{n\theta}(k) dk \\ &\quad \times \int_0^{2\pi} d\varphi \int_0^\pi \sin \vartheta d\vartheta \frac{k_z^2}{k^2}, \end{aligned} \quad (\text{A14})$$

where we use the spherical coordinates (k, ϑ, φ) in the \mathbf{k} -space. For the integration over angles in \mathbf{k} -space, we use the following integral:

$$\int_0^{2\pi} d\varphi \int_0^\pi \sin \vartheta d\vartheta \frac{k_i k_j}{k^2} = \frac{4\pi}{3} \delta_{ij}. \quad (\text{A15})$$

Therefore, for large Péclet numbers, this correlation function is given by

$$\langle n(t, \mathbf{x}) \Delta^{-1} \nabla_z^2 \theta(t, \mathbf{x}) \rangle \approx \frac{1}{3} \langle n \theta \rangle. \quad (\text{A16})$$

Now, we determine the correlation function $\langle n \Delta^{-1} \nabla_z^2 \theta \rangle$ for an anisotropic turbulence,

$$\begin{aligned} \langle n(t, \mathbf{x}) \Delta^{-1} \nabla_z^2 \theta(t, \mathbf{x}) \rangle &= \int_{\tilde{\ell}_z}^\infty dk_z \int_{\tilde{\ell}_h}^\infty k_h dk_h \\ &\times \int_0^{2\pi} d\phi \left(1 - \frac{1}{1 + k_z^2/k_h^2} \right) \langle n(\mathbf{k}) \theta(-\mathbf{k}) \rangle, \end{aligned} \quad (\text{A17})$$

where we use the cylindrical coordinates (k_h, ϕ, k_z) in \mathbf{k} -space, and $\tilde{\ell}_z$ and $\tilde{\ell}_h$ are the correlation lengths of the correlation function $\langle n(t, \mathbf{x}) \theta(t, \mathbf{y}) \rangle$ in the vertical and horizontal directions. For strongly anisotropic turbulence, i.e., when $\tilde{\ell}_z \ll \tilde{\ell}_h$, the contribution of the first term on the right-hand side of Eq. (A17) is dominant so that

$$\langle n(t, \mathbf{x}) \Delta^{-1} \nabla_z^2 \theta(t, \mathbf{x}) \rangle \approx \langle n \theta \rangle. \quad (\text{A18})$$

Therefore, $\langle n(t, \mathbf{x}) \Delta^{-1} \nabla_z^2 \theta(t, \mathbf{x}) \rangle = C_* \langle n \theta \rangle$, where C_* varies from 0.3 to 1 depending on the degree of anisotropy of turbulence.

When $i = x, y$, the correlation function $\langle n \Delta^{-1} \nabla_z \nabla_i \theta \rangle$ vanishes in isotropic turbulence. Equations (A7), (A16), and (A18) yield the expression for the correlation term $Q_i^{(n)}$ as

$$Q_i^{(n)} = -\frac{C_D}{2} \beta \tau_i e_i F_j^{(n)} \nabla_j \bar{\Theta} + \beta \nabla_i \langle n \Delta^{-1} \nabla_z \theta \rangle, \quad (\text{A19})$$

where \mathbf{e} is the vertical unit vector and $C_D = C_{n\theta} (1 + C_*)$ is an empirical dimensionless constant.

DATA AVAILABILITY

Data sharing is not applicable to this article as no new data were created or analyzed in this study.

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