

## Deviations from unity of the ratio of the turbulent Schmidt to Prandtl numbers in stratified atmospheric flows over water surfaces

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Expressions for the ratio of the turbulent Schmidt ( $Sc_t$ ) to Prandtl ( $Pr_t$ ) numbers are derived for an idealized atmospheric surface layer flow over water surfaces. Conditions where the ansatz  $Sc_t/Pr_t \approx 1$  are then discussed. It is shown that  $Sc_t/Pr_t \approx 1$  is consistent with the active role of temperature in turbulence generation or destruction even when perfect similarity between turbulent transport of heat and water vapor is absent.

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### I. INTRODUCTION

Despite their ad hoc introduction some 140 years ago [1], eddy diffusivity and eddy viscosity ( $K_m$ ) remain fruitful concepts in turbulence research. They qualify as the first successful application of renormalization group (RNG) methods, arguably well before RNG's formal development in quantum field theory [2]. Their use has made it possible to measure and model turbulent fluxes in natural systems operating at Reynolds numbers that are simply too large to resolve in direct numerical simulations. A case in point is the 1926 seminal work of the physicist Ira Bowen [3,4], who determined lake evaporation ( $E$ ) and heat conduction ( $H$ ) using the concept of eddy diffusivity and similarity between heat and water vapor transport. Bowen's original derivation assumed the ratio of eddy diffusivity for heat ( $K_T$ ) to water vapor ( $K_q$ ) or equivalently the ratio of the turbulent Schmidt ( $Sc_t = K_m/K_q$ ) to Prandtl ( $Pr_t = K_m/K_T$ ) numbers be unity. This assumption is now routinely employed in climate and weather forecasting models [5,6] and is justified using similarity in heat and water vapor sources and sinks at the water surface along with similarity in turbulent transport characteristics [7]. There is renewed interest in deviations from unity in  $Sc_t/Pr_t$  given the proliferation of remote-sensing products aimed at inferring the Bowen ratio  $\beta = H/E$  from radiometric mean surface ( $T_s$ ) measurements [8–13]. This inference of  $\beta$  from  $T_s$  and theoretical limits on  $\beta$  at a given  $T_s$  routinely assumes  $Sc_t/Pr_t = 1$  [14–18] as in the original work of Bowen.

To be clear, this assumption cannot be entirely correct [19–22] as temperature is an active scalar (i.e., a scalar that produces or dissipates turbulent kinetic energy). Water vapor concentration turbulent fluctuations also impact air density, though this impact is usually small when compared to their temperature counterparts. Measurements of the correlation coefficient between turbulent air temperature and water vapor concentration fluctuations  $R_{Tq}$  above large water bodies also challenge the assumption  $Sc_t/Pr_t = 1$ . The  $R_{Tq}$  is used as a so-called signature of scalar similarity but deviations from unity are routinely reported [22–24]. Over land, it has been known for some time that  $K_T$  and  $K_q$  can differ and the difference partly depends on the thermal stratification in the atmosphere [25,26]. Moreover, in the presence of horizontal advection or entrainment,  $K_T$  and  $K_q$  also differ [27–32] with some experiments reporting  $K_T/K_q > 5$  [33]. Nonetheless, the weighty Kansas experiment over flat and uniform surface [34] suggests that  $K_T \approx K_q$  across a wide range of

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atmospheric stability regimes [35], which was also confirmed by other extensive experiments [36]. Studies over large water bodies also appear mixed with regards to  $K_T = K_q$  when analyzed in the context of  $R_{Tq}$ . Some experiments favor near-perfect similarity [37] while others report nontrivial deviations from unity [38,39] in  $|R_{Tq}|$ . Likewise, deviations in  $|R_{Tq}|$  from unity over oceans have also been reported in several large-scale experiments [40]. The reason why  $R_{Tq}$  deviates from unity near the surface, even in the absence of horizontal advection, is partly connected with scalar dissimilarity in entrainment at the top of the atmospheric boundary layer, as confirmed by a large corpus of experiments and simulations [24,30,31,41,42]. The apparent contradiction in setting  $K_T/K_q \approx 1$  despite  $|R_{Tq}| < 1$  and the fact that air temperature is an active scalar are examined here. The goal is to explain maximum deviations in  $K_T/K_q$  from unity due to these two aforementioned effects. Advection, subsidence, and nonstationary conditions are not considered as they act above and beyond these cases. Advective conditions, which are prevalent in some experiments [27–29,33,43], are more difficult to discuss because turbulent fluxes are no longer constant with height  $z$  and the advective time scale may be comparable with the equilibration time scale, raising questions as to whether gradient-diffusion closure (or K theory) applies [44,45].

## II. THEORY

### A. Definitions

The idealized setup by Bowen is first considered [3,4]. This setup assumes a stationary and planar-homogeneous high Reynolds number air flow at some height  $z$  over a uniform water surface in the absence of any subsidence. The net available energy  $Q_n$  at the air-water interface is partitioned into sensible  $H$  and latent  $E$  heat fluxes so that  $Q_n = E + H$ . By definition [3,4],  $\beta = H/E$  and  $E = Q_n(1 + \beta)^{-1}$ . It is further assumed that  $\beta \neq -1$  and  $|E| > 0$ . If molecular diffusion coefficients for heat and water vapor in air are ignored relative to their turbulent counterparts ( $K_T$  and  $K_q$ ), then the actual evaporation is given by the turbulent flux  $E = L_v \overline{w'q'}$  and the sensible heat flux is given by  $H = \rho C_p \overline{w'T'}$ , where  $L_v$  is the latent heat of vaporization,  $\rho$  is the mean air density,  $C_p$  is the specific heat capacity of dry air at constant pressure,  $w'$  is the turbulent vertical velocity excursion from the mean state  $\overline{w} = 0$  (no subsidence),  $T'$  and  $q'$  are turbulent air temperature and water vapor concentration excursions from their mean  $\overline{T}(z)$  and  $\overline{q}(z)$ , and an overline indicates Reynolds averaging. Using K theory, the turbulent scalar fluxes are given by

$$\overline{w'q'} = -K_q \frac{d\overline{q}}{dz}; \quad \overline{w'T'} = -K_T \frac{d\overline{T}}{dz}. \quad (1)$$

Likewise, the kinematic turbulent stress is given by

$$\frac{\tau_t}{\rho} = -\overline{w'u'} = u_*^2 = K_m \frac{d\overline{U}}{dz}, \quad (2)$$

where  $u'$  are turbulent excursions from the mean longitudinal velocity  $\overline{U}$ ,  $\overline{w'u'}$  is the turbulent momentum flux,  $K_m$  is assumed to be much larger than the molecular viscosity of air  $\nu$ , and  $u_*$  is the friction or shear velocity. Throughout, the Reynolds number  $\text{Re}_* = u_* z / \nu$  is assumed to be sufficiently large to ignore viscous effects. This assumption is plausible in the atmospheric surface layer (ASL) over water surfaces, where  $u_* \sim 0.1 \text{ m s}^{-1}$ ,  $z \sim 1 \text{ m}$ , and  $\nu \sim 1.5 \times 10^{-5} \text{ m}^2 \text{ s}^{-1}$ . Exploring how  $K_T/K_q$  varies for such idealized flow is equivalent to evaluating how  $\text{Sc}_t/\text{Pr}_t$  varies with atmospheric stability and other bulk flow variables (e.g., boundary layer height).

As is conventional in the analysis of ASL flows, dimensionless quantities for the first and second moments are considered and are defined as [46,47]

$$\frac{d\overline{T}}{dz} = \frac{T_*}{\kappa z} \phi_h(\zeta); \quad \frac{d\overline{q}}{dz} = \frac{q_*}{\kappa z} \phi_v(\zeta); \quad \frac{d\overline{U}}{dz} = \frac{u_*}{\kappa z} \phi_m(\zeta); \quad (3)$$

$$\frac{\sigma_w}{u_*} = \phi_{ww}(\zeta); \quad \frac{\sigma_T}{T_*} = \phi_{TT}(\zeta); \quad \frac{\sigma_q}{q_*} = \phi_{qq}(\zeta); \quad (4)$$

where  $\phi_h$ ,  $\phi_v$ , and  $\phi_m$  are referred to as stability correction functions for heat, water vapor, and momentum, respectively;  $\sigma_T^2 = \overline{T'T'}$ ;  $\sigma_q^2 = \overline{q'q'}$ ;  $\sigma_w^2 = \overline{w'w'}$ ; and  $T_*$ ,  $q_*$ , the stability parameter  $\zeta$ , and the Obukhov length  $L$  [48] are, respectively, given as

$$T_* = -\frac{\overline{w'T'}}{u_*}; \quad q_* = -\frac{\overline{w'q'}}{u_*}; \quad \zeta = \frac{z}{L}; \quad L = \frac{u_*^2}{\kappa\beta_o T_*}, \quad (5)$$

where  $\kappa \approx 0.4$  is the von Kármán constant,  $\beta_o = g/T_a$  is the buoyancy parameter, and  $g = 9.81 \text{ m s}^{-2}$  is the gravitational acceleration. Here, unstable, stable, and near-neutral atmospheric stability conditions are associated with  $\zeta < 0$ ,  $\zeta > 0$ , and  $\zeta \approx 0$ , respectively. A  $\zeta \approx -1$  signifies a height at which mechanical production of turbulent kinetic energy (TKE) is commensurate with buoyant production of TKE. In the definition of  $L$ , it was assumed that water vapor concentration corrections are small relative to their temperature counterpart. Based on these definitions,

$$\frac{K_T}{K_q} = \frac{\text{Sc}_t}{\text{Pr}_t} = \frac{\phi_v(\zeta)}{\phi_h(\zeta)}. \quad (6)$$

To illustrate the utility of  $K_T/K_q$  to the plethora of problems earlier mentioned, it is noted that

$$\left(\frac{K_T}{K_q}\right) \frac{\frac{d\overline{T}}{dz}}{\frac{d\overline{q}}{dz}} = \frac{\sigma_w \sigma_T R_{wT}}{\sigma_w \sigma_q R_{wq}}, \quad (7)$$

which when combined with the similarity theory expressions yields

$$\frac{\phi_{TT}(\zeta)}{\phi_{qq}(\zeta)} = \left(\frac{R_{wT}}{R_{wq}}\right)^{-1}. \quad (8)$$

The quantity  $R_{wT}/R_{wq}$  is labeled as the relative transport efficiency of heat to water vapor [22,49]. With these expressions,

$$\beta = \frac{H}{E} = \frac{\rho C_p}{L_v} \left(\frac{K_T}{K_q}\right) \frac{\frac{d\overline{T}}{dz}}{\frac{d\overline{q}}{dz}} = \beta_{ap} \left(\frac{K_T}{K_q}\right), \quad (9)$$

where

$$\beta_{ap} \approx \frac{\rho C_p}{L_v} \frac{\overline{T}_s - \overline{T}(z)}{q(\overline{T}_s) - \overline{q}(z)}, \quad (10)$$

is mainly used to link remotely sensed  $\overline{T}_s$  to  $\beta$  given that the (saturated) water vapor concentration at the water surface  $q(\overline{T}_s)$  can be predicted from  $\overline{T}_s$  using the Clausius-Clapeyron expression. As earlier noted, if similarity of heat and water vapor transport is invoked,  $\text{Sc}_t = \text{Pr}_t$ ,  $K_T = K_q$ , and  $\beta_{ap} = \beta$  as originally assumed in the 1926 manuscript of Bowen. To relax this assumption, a model is required to explain how  $K_T/K_q$  deviates from unity and is explored above water surfaces. Specifically, constraints on the magnitude of  $K_T/K_q$  and atmospheric stability regimes that elicit maximum deviations from unity are the sought-after outcomes. The trivial case when  $R_{Tq} = \overline{T'q'}/(\sigma_T \sigma_q) = 1$  (perfect similarity) is not repeated here because it directly leads to  $R_{wT} = R_{wq}$  and  $K_T = K_q$  as discussed elsewhere [7]. For this reason, it is assumed through out that  $|R_{Tq}| < 1$ . It is noted that  $|R_{Tq}| < 1$  places minor constraints on the magnitude of  $R_{wT}/R_{wq}$  as can be shown from the Gram determinant inequality [50] discussed elsewhere [39,51]. Hence, the product  $|R_{Tq} R_{wT}/R_{wq}|$  can be unity or exceed unity even when  $|R_{Tq}| < 1$ .

### B. Bringing the eddies into $\text{Sc}_t/\text{Pr}_t$

To arrive at expressions for  $\text{Sc}_t/\text{Pr}_t$ , contributions of various wave numbers  $k$  associated with the spectra of turbulence are considered and are given as

$$\frac{K_T}{K_q} = \frac{\rho C_p}{L_v} \frac{\frac{d\overline{q}}{dz} \int_0^\infty F_{wT}(k) dk}{\frac{d\overline{T}}{dz} \int_0^\infty F_{wq}(k) dk}, \quad (11)$$

where  $F_{wT}(k)$  and  $F_{wq}(k)$  are the cospectra for heat and water vapor fluxes, respectively, and  $k$  is interpreted as the 1-D wave number along  $\bar{U}$ . It can be shown that for stationary and planar homogeneous high Reynolds number flow in the absence of subsidence, these cospectra at any  $k$  can be approximated by [52–57]

$$F_{wT}(k) = \frac{-(1 - C_I) \frac{d\bar{T}}{dz} F_{ww}(k) + (1 - 2\alpha_I) \beta_o F_{TT}(k)}{(1 + \text{Pr}_m^{-1}) \nu k^2 + A_R \tau(k)^{-1}}, \quad (12)$$

and

$$F_{wq}(k) = \frac{-(1 - C_I) \frac{d\bar{q}}{dz} F_{ww}(k) + (1 - 2\alpha_I) \beta_o F_{Tq}(k)}{(1 + \text{Sc}_m^{-1}) \nu k^2 + A_R \tau(k)^{-1}}, \quad (13)$$

where  $A_R$ ,  $C_I$ , and  $\alpha_I$  are constants related to the Rotta closure model. Specifically,  $C_I$  is related to the isotropization of the production term and a value  $C_I = 3/5$  has been predicted from rapid distortion theory [58]. An  $\alpha_I = 1/3$  is predicted for isotropic turbulence [59] though the effects of  $\zeta$  on its magnitude remain uncertain, and  $A_R = 1.8$  is the Rotta constant associated with the term describing the slow part of the pressure-scalar interaction as discussed elsewhere [60,61]. The  $\tau(k) = \epsilon^{-1/3} k^{-2/3}$  is a wave-number-dependent relaxation time scale [62–65] that varies with the mean dissipation rate of TKE,  $\epsilon$ ,  $F_{ww}(k)$  and  $F_{TT}(k)$  are the vertical velocity and air temperature spectra, respectively, satisfying the normalizing properties  $\int_0^\infty F_{ww}(k) dk = \sigma_{ww}^2$  and  $\int_0^\infty F_{TT}(k) dk = \sigma_{TT}^2$ , and  $F_{Tq}(k)$  is the temperature-humidity cospectrum satisfying the normalizing property  $\int_0^\infty F_{Tq}(k) dk = \overline{T'q'}$ , and  $\text{Pr}_m \approx 0.7$  and  $\text{Sc}_m \approx 0.6$  are the molecular Prandtl and Schmidt numbers in air at standard temperature and pressure. Defining the Kolmogorov microscale as  $\eta_{ko} = (\nu^3/\epsilon)^{1/4}$  [58,66], it directly follows that  $(A_R \epsilon^{1/3} k^{2/3}) \gg [(1 + \text{Pr}_m^{-1}) \nu k^2]$  when  $k \eta_{ko} \ll [A_R / (1 + \text{Pr}_m^{-1})]^{3/4} \approx 0.7$ . This condition implies that the molecular terms are only comparable to the pressure-scalar interaction term when  $k \eta_{ko}$  is of order unity. Such small scales do not contribute appreciably to turbulent scalar or momentum fluxes and are ignored thereafter [58] due the high  $\text{Re}_*$  characterizing ASL flows (i.e.,  $\eta_{ko}/z \ll 1$ ). In terms of arbitrary spectral shapes, the wave-number integrated budget equation models are given by

$$\overline{w'T'} = \frac{1 - C_I}{A_R} \frac{d\bar{T}}{dz} I_1 \left[ -1 + \frac{(1 - 2\alpha_I) \beta_o I_2}{(1 - C_I) \frac{d\bar{T}}{dz} I_1} \right] \quad (14)$$

and

$$\overline{w'q'} = \frac{1 - C_I}{A_R} \frac{d\bar{q}}{dz} I_1 \left[ -1 + \frac{(1 - 2\alpha_I) \beta_o I_3}{(1 - C_I) \frac{d\bar{q}}{dz} I_1} \right], \quad (15)$$

where the integrals are given as

$$I_1 = \int_0^\infty \tau(k) F_{ww}(k) dk, \quad (16)$$

$$I_2 = \int_0^\infty \tau(k) F_{TT}(k) dk,$$

$$I_3 = \int_0^\infty \tau(k) F_{Tq}(k) dk. \quad (17)$$

The cospectrum can be linked to  $F_{TT}(k)$  and the water vapor concentration spectrum  $F_{qq}(k)$  using  $F_{Tq}(k) = \text{Coh}(T, q) [F_{TT}(k) F_{qq}(k)]^{1/2}$ , where  $\text{Coh}(k)$  is the coherence spectrum. Regardless of the

spectral and cospectral shapes, these definitions yield

$$\frac{K_T}{K_q} = \frac{\left[-1 + \frac{(1-2\alpha_I)\beta_o I_2}{(1-C_I)\frac{dT}{dz} I_1}\right]}{\left[-1 + \frac{(1-2\alpha_I)\beta_o I_3}{(1-C_I)\frac{dq}{dz} I_1}\right]}. \quad (18)$$

As earlier mentioned, the numerical value for  $\alpha_I$  appears uncertain in stratified high-Reynolds-number flows with  $\alpha_I = 0$  suggested for stable flows [55] and  $\alpha_I = 1/2$  estimated from large eddy simulation (LES) studies of the convective boundary layers [59,67]. If  $\alpha_I$  increases from its isotropic value of  $1/3$  to  $1/2$ , then  $K_T/K_q = 1$  irrespective of any dissimilarity between heat and water vapor transport or stability regime.

### C. Linking spectral shapes to $K_T/K_q$

Three cases are now considered with regards to the shapes of  $\tau(k)$ ,  $F_{ww}(k)$ ,  $F_{TT}(k)$ , and  $F_{Tq}(k)$  that impact  $I_1$ ,  $I_2$ , and  $I_3$ . These three cases are ordered from simple to complex, with the case 1 lumping all the effects of turbulence into a master time scale as common to higher-order Reynolds-averaged Navier-Stokes (RANS) closure models. The most complex case, case 3, accounts for all turbulent scales using realistic energy spectra derived from field measurements over lakes. Case 2 is intermediate and assumes all turbulent spectra follow Kolmogorov scaling [68] for all  $1/h_o < k < \infty$ , where  $h_o$  may be interpreted as the largest turbulent scale in the flow.

*Case 1: The constant  $\tau$ .* In this case,  $\tau(k)$  is replaced by a single effective relaxation time scale  $\tau_{\text{eff}}$  acting equally on all  $k$ . This case highlights many common features between this approach and higher-order closure models that assign a single length or time scale to all turbulent eddies. With  $\tau(k) = \tau_{\text{eff}}$  being independent of  $k$ , and when integrating across all  $k$  leads to  $I_1 = \tau_{\text{eff}}\sigma_w^2$ ,  $I_2 = \tau_{\text{eff}}\sigma_T^2$ , and  $I_3 = \tau_{\text{eff}}\overline{T'q'}$ . Expressed in terms of stability correction functions, this modeled  $K_T/K_q$  reduces to

$$\frac{K_T}{K_q} = \frac{1 - \frac{1-2\alpha_I}{1-C_I} \frac{\varsigma}{\phi_h(\varsigma)} \left(\frac{\phi_{TT}(\varsigma)}{\phi_{ww}(\varsigma)}\right)^2}{1 - \frac{1-2\alpha_I}{1-C_I} R_{Tq} \frac{\varsigma}{\phi_v(\varsigma)} \left[\frac{\phi_{qq}(\varsigma)\phi_{TT}(\varsigma)}{(\phi_{ww}(\varsigma))^2}\right]}. \quad (19)$$

The similarity theory results for  $\phi_v(\varsigma)$  and  $\phi_{qq}(\varsigma)$  in the above expression are linked to their temperature counterparts  $\phi_h(\varsigma)$  and  $\phi_{TT}(\varsigma)$  through  $R_{Tq}$  and  $R_{wT}/R_{wq}$  to yield

$$\frac{K_T}{K_q} = \frac{1 - \frac{1-2\alpha_I}{1-C_I} \frac{\varsigma}{\phi_h(\varsigma)} \left(\frac{\phi_{TT}(\varsigma)}{\phi_{ww}(\varsigma)}\right)^2}{1 - R_{Tq} \left(\frac{K_T}{K_q}\right)^{-1} \left(\frac{R_{wT}}{R_{wq}}\right)^{\frac{1-2\alpha_I}{1-C_I}} \frac{\varsigma}{\phi_h(\varsigma)} \left(\frac{\phi_{TT}(\varsigma)}{\phi_{ww}(\varsigma)}\right)^2}. \quad (20)$$

This solution can be recast as

$$\frac{K_T}{K_q} = \frac{1 - \Gamma_1(\varsigma)}{1 - \left(\frac{K_T}{K_q}\right)^{-1} \left(\frac{R_{wT}}{R_{wq}}\right) R_{Tq} \Gamma_1(\varsigma)}, \quad (21)$$

where the function

$$\Gamma_1(\varsigma) = \frac{1 - 2\alpha_I}{1 - C_I} \frac{\varsigma}{\phi_h(\varsigma)} \left(\frac{\phi_{TT}(\varsigma)}{\phi_{ww}(\varsigma)}\right)^2. \quad (22)$$

Solving this expression for  $K_T/K_q$  yields

$$\frac{K_T}{K_q} = \frac{\text{Sc}_t}{\text{Pr}_t} = 1 + \Gamma_1(\varsigma) \left[ \left(\frac{R_{wT}}{R_{wq}}\right) R_{Tq} - 1 \right]. \quad (23)$$

This expression is identical to earlier ones derived from standard higher-order closure models [19,21] when the  $(1 - 2\alpha_I)(1 - C_I)^{-1}$  multiplier in  $\Gamma_1$  is replaced by  $1/2$ . The  $(1 - 2\alpha_I)(1 - C_I)^{-1}$  multiplier originates from the isotropization of the production term here. The  $\Gamma_1(\varsigma)$  is purposely

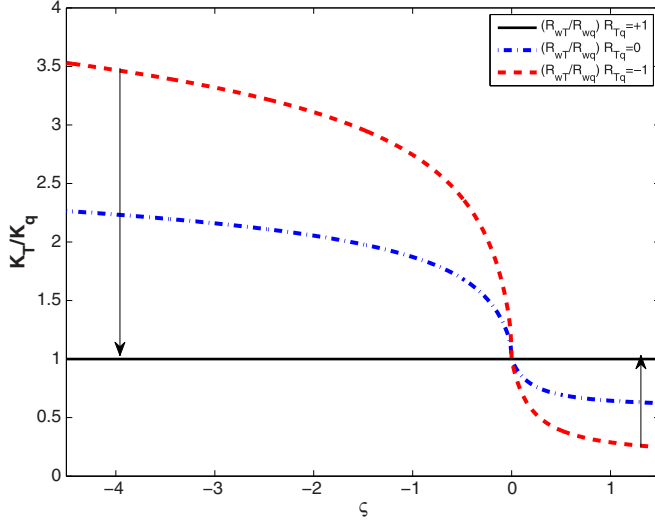


FIG. 1. Predicted variations of  $K_T/K_q$  with  $\zeta$  for case 1 using Eq. (23) for  $(R_{wT}/R_{wq})R_{Tq} = +1$ ,  $|(R_{wT}/R_{wq})R_{Tq}| = 0$ , and  $(R_{wT}/R_{wq})R_{Tq} = -1$  with  $\alpha_I = 1/3$ . Unstable and stable atmospheric stability conditions are delineated by  $\zeta < 0$  or  $\zeta > 0$ , respectively. Arrows indicate increasing  $(R_{wT}/R_{wq})R_{Tq}$  from  $-1$  to  $+1$ .

formulated to be independent of water vapor statistics and all the water vapor effects on  $K_T/K_q$  are included in  $(R_{wT}/R_{wq})R_{Tq}$ . The function satisfies the condition  $\Gamma_1(0) = 0$ . The model here predicts a  $K_T/K_q = 1$  when (1)  $|\zeta| \rightarrow 0$  (i.e., near-neutral conditions) or when (2)  $(R_{wT}/R_{wq})R_{Tq} = 1$  (perfect similarity between heat and water vapor transport as discussed elsewhere [7]). While the expression here is only sensitive to the product  $(R_{wT}/R_{wq})R_{Tq}$ , the trivial case where  $R_{Tq} = 1$  resulting in  $R_{wT}/R_{wq} = 1$  recovers  $K_T/K_q = 1$  irrespective of  $I_1$ ,  $I_2$ , and  $I_3$ . The expression also delineates two other dynamically interesting regimes. The first is when  $|(R_{wT}/R_{wq})R_{Tq}| = 0$  and the second regime is when  $(R_{wT}/R_{wq})R_{Tq} = -1$ . To illustrate the possible range of variability in  $K_T/K_q$  in these two regimes, standard ASL values for  $\phi_{ww}$ ,  $\phi_{TT}$ , and  $\phi_h$  are used in Fig. 1 predicting  $K_T/K_q$ .

For unstable conditions,  $\zeta < 0$ :

$$\phi_{ww}(\zeta) = A_{ww} (1 - 3\zeta)^{\frac{1}{3}}; \quad \phi_{TT}(\zeta) = 0.95(\zeta)^{-1/3}; \quad (24)$$

$$\phi_h(\zeta) = (1 - 16\zeta)^{-1/2}. \quad (25)$$

For stable conditions,  $\zeta > 0$ :

$$\phi_{ww}(\zeta) = A_{ww} = 1.25; \quad \phi_{TT}(\zeta) = A_{TT} = 2; \quad (26)$$

$$\phi_h(\zeta) = 1 + b\zeta; \quad b = 5. \quad (27)$$

It is evident that  $K_T/K_q \geq 1$  are predicted for unstable conditions and  $K_T/K_q \leq 1$  for stable conditions when  $R_{wT}/R_{wq}R_{Tq} \neq 1$ .

With this background and noting the association between  $K_T/K_q$  and  $(R_{wT}/R_{wq})R_{Tq}$ , it is instructive to ask how  $(R_{wT}/R_{wq})R_{Tq}$  varies with atmospheric stability above water surfaces when  $|R_{Tq}| < 1$ . Figure 2 presents these variations using published data above two large lakes characterized by different climatic regimes and marine boundary layers. It is clear that much of the variations occur in near-neutral conditions where Eq. (23) predicts  $K_T \approx K_q$  no matter what values  $(R_{wT}/R_{wq})R_{Tq}$

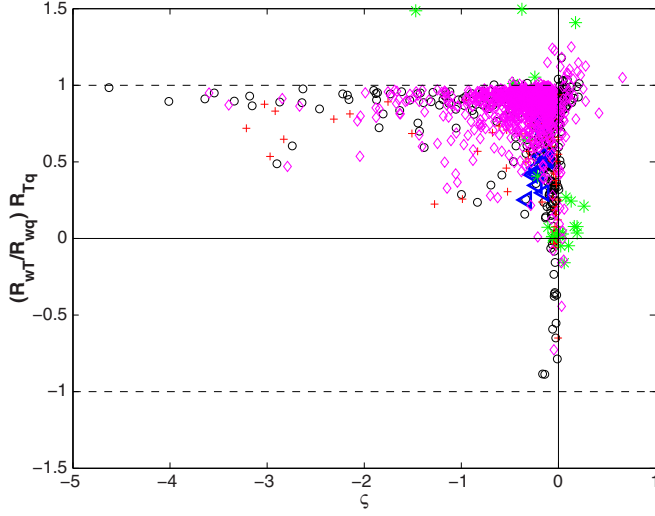


FIG. 2. Variation of measured  $(R_{wT}/R_{wq})R_{Tq}$  with measured atmospheric stability parameter  $\zeta$  above Lake Lemman, Switzerland (open circles), and Lake Kinneret, Israel (pluses), both described elsewhere [39], a marine boundary layer (stars) where heat and water vapor fluxes did not vary by more than 20% with height from the Riso Air-Sea Experiment (RASEX) described elsewhere [41], and a large inland water body in Mississippi (Ross Barnett Reservoir), USA (diamond), described elsewhere [69,70]. For reference, the 1969 San Diego and Barbados ocean experiments (triangles) are also shown (taken from Table 1 from Phelps and Pond [40]).

takes on. For unstable conditions,  $(R_{wT}/R_{wq})R_{Tq}$  tends to be between 0.5 and 1.0, suggesting a  $K_T/K_q \geq 1$ . Again, few instances are noted when  $-1 < (R_{wT}/R_{wq})R_{Tq} < 0$ , but those instances appear to be rare and still associated with near-neutral conditions when Eq. (23) predicts  $K_T \approx K_q$  due to  $\Gamma_1(0) \approx 0$ . For mildly stable conditions,  $(R_{wT}/R_{wq})R_{Tq} \approx +1$ , again suggesting that  $K_T \approx K_q$ . When interpreting Eq. (23) in this context, the data featured here suggest that much uncertainty in  $K_T/K_q$  appears to be associated with mildly unstable or mildly stable regimes, where  $(R_{wT}/R_{wq})R_{Tq}$  varies appreciably and  $\Gamma_1(\zeta)$  remains finite.

*Case 2: Inertial spectra.* While imposing a single effective relaxation time recovers predictions from earlier closure models [19,21,22], it is unrealistic. To illustrate, consider the case when the spectra of turbulence are assumed to be inertial [71] and follow Kolmogorov [68] scaling from  $k = 1/h_o$  to  $k \rightarrow \infty$ , where  $h_o$  is the largest scale of turbulence. For these idealized shapes (and for  $Sc_m \approx Pr_m \approx 1$ ), the spectra  $F_{ww}(k) = C_{ow}\epsilon^{2/3}k^{-5/3}$ ,  $F_{TT}(k) = C_T\epsilon^{-1/3}N_Tk^{-5/3}$ ,  $\epsilon \equiv -\overline{u'w'}(d\overline{U}/dz) + \beta_o\overline{w'T'}$  are derived from a TKE budget that is in equilibrium [72,73],  $N_T \approx -\overline{w'T'}(d\overline{T}/dz)$  is the half-variance temperature dissipation rate,  $C_{ow} \approx 0.65$  is the Kolmogorov constant for the vertical velocity component [74], and  $C_T \approx 0.8$  is the Kolmogorov-Obukhov-Corrsin constant for the temperature spectrum [36,75–77]. For these assumed spectra,  $F_{wT} \sim k^{-7/3}$  expected in boundary layers [58,78–80]. If  $\tau(k) = \tau_{\text{eff}}$  as previously considered, then  $F_{wT} \sim k^{-5/3}$ , an unconventional cospectral scaling for the inertial subrange. For the second case then, the  $\tau(k) = k^{-2/3}\epsilon^{-1/3}$  is considered instead of  $\tau_{\text{eff}}$ . For reference, the vertical velocity, air temperature, and water vapor concentration spectra are all assumed to follow inertial subrange scaling laws unaffected by intermittency, large-scale or boundary effects, viscous cutoff, or bottlenecks [81]. For these idealized spectral shapes, and upon integration across all scales bounded by  $1/h_o \leq k \leq \infty$  yields for  $I_1$  and  $I_2$  the following:

$$I_1 = \frac{3}{4}C_{ow}\epsilon^{1/3}h_o^{4/3}, \quad I_2 = \frac{3}{4}C_T\epsilon^{-2/3}N_T h_o^{4/3}. \quad (28)$$

To evaluate  $I_3$ , assumptions about the shape of  $F_{Tq}(k)$  and  $F_{qq}(k)$  are required. Here,  $F_{qq}(k) = C_q\epsilon^{-1/3}N_qk^{-5/3}$ ,  $C_q \approx C_T$  [36] is the Kolmogorov constant for the water vapor concentration

spectrum in the inertial subrange and  $N_q$  is the half-variance dissipation rate of  $q'$ . A model of maximum simplicity is to set the coherence spectrum a constant  $A_{T,q}$  but constrained by the condition  $|A_{T,q}| < 1$  to ensure  $|R_{Tq}| < 1$  at all  $1/h_o < k < \infty$  so that

$$F_{Tq}(k) = A_{T,q}(C_T C_q)^{1/2} \epsilon^{-1/3} (N_T N_q)^{1/2} k^{-5/3}, \quad (29)$$

where  $A_{T,q}$  is determined from the normalizing property  $\int_{1/h_o}^{\infty} F_{Tq}(k) dk = \overline{T'q'}$  to yield

$$A_{T,q} = \frac{2}{3} \frac{\overline{T'q'}}{(C_T C_q)^{1/2} \epsilon^{-1/3} (N_T N_q)^{1/2} h_o^{2/3}}. \quad (30)$$

With this  $A_{T,q}$  estimate,  $F_{Tq}(k) = (2/3) \overline{T'q'} h_o^{-2/3} k^{-5/3}$  and  $I_3$  is now given by

$$I_3 = \frac{1}{2} \overline{T'q'} \epsilon^{-1/3} h_o^{2/3}. \quad (31)$$

There is some support for a near-constant  $\text{Coh}(k)$  shape over land and water [40,82] when  $kz < 1$ . As expected, this assumption fails when  $kz \gg 1$  as  $\text{Coh}(T, q) \rightarrow 0$  due to the isotropic nature of small-scale eddies. These estimates of  $I_1$ ,  $I_2$ , and  $I_3$  result in

$$\frac{K_T}{K_q} = \frac{1 + \Gamma_2(\zeta)}{1 + \left(\frac{K_T}{K_q}\right)^{-1} R_{Tq} \frac{R_{wT}}{R_{wq}} \Gamma_2(\zeta) \theta_2(\zeta)}, \quad (32)$$

where

$$\Gamma_2(\zeta) = \frac{1 - 2\alpha_I}{1 - C_I} \frac{C_T}{C_{ow}} \frac{\zeta}{\phi_m(\zeta) - \zeta}, \quad (33)$$

$$\theta_2(\zeta) = \frac{2}{3} \frac{1}{C_T} \frac{(\phi_m(\zeta) - \zeta)^{1/3} (\phi_{TT}(\zeta))^2}{\phi_h(\zeta)} \left(\frac{\kappa z}{h_o}\right)^{2/3}. \quad (34)$$

Solving for  $K_T/K_q$  leads to

$$\frac{K_T}{K_q} = 1 + \Gamma_2(\zeta) \left[ R_{Tq} \frac{R_{wT}}{R_{wq}} \theta_2(\zeta) - 1 \right]. \quad (35)$$

As before,  $\Gamma_2(0) = 0$  and corrections to  $K_T/K_q$  are only significant when  $|\zeta| > 0$  (i.e., thermally stratified flow). However, this solution differs from earlier outcomes in several ways: (1) it shows that  $K_T/K_q$  is influenced by  $\phi_m(\zeta)$  whereas the previous solutions were influenced by  $\phi_{ww}(\zeta)$ , (2) the multiplier  $\theta_2$  is not unity and itself varies with atmospheric stability conditions whereas previous solutions suggest  $\theta_2 = 1$ , and (3)  $z/h_o$  emerges as a significant quantity that need not be a constant when  $h_o$  scales with the ABL height (instead of  $z$  as in previous solutions). For example, when  $z/h_o \ll 1$ ,  $\theta_2 \approx 0$ , and  $K_T/K_q$  becomes decoupled from any dissimilarity in scalar transport characterized by  $R_{Tq}(R_{wT}/R_{wq})$  but still varies with  $\zeta$ . This result, which only applies for  $|R_{Tq}| < 1$ , could not have been foreshadowed by earlier models.

*Case 3: Realistic spectra.* The third case considers realistic spectral shapes in the ASL for  $F_{ww}(k)$ ,  $F_{TT}(k)$ , and  $F_{qq}(k)$  instead of inertial subrange scaling, again assuming  $|R_{Tq}| < 1$ . The spectral shapes to be specified are approximations to measurements reported in Fig. 3. For analytical tractability, only the essential features of these measured spectra in Fig. 3 are described: A wave number  $k_a = 1/z$  delineates large scales from inertial scale eddies in  $w'$  so that  $F_{ww}(k) = C_{ow} \epsilon^{2/3} k_a^{-5/3}$  represents the spectrum for  $kz < 1$  (i.e., a flat spectrum) and  $F_{ww}(k) = C_{ow} \epsilon^{2/3} k^{-5/3}$  describes the spectrum for  $kz > 1$ , an oversimplification here. Likewise,  $\tau(k) = \epsilon^{-1/3} k_a^{-2/3}$  for  $kz < 1$  and  $\tau(k) = \epsilon^{-1/3} k^{-2/3}$  for  $kz > 1$ . With regards to  $F_{TT}(k)$ , three regimes are identified: The inertial regime with  $F_{TT}(k) = C_T \epsilon^{-1/3} N_T k^{-5/3}$  for  $kz > 1$  as with  $F_{ww}(k)$ , the production regime given as  $F_{TT}(k) = C_p T_*^2 k^{-1}$  for  $h_o^{-1} < k < z^{-1}$ , where upon matching this regime to the inertial at  $k_a z = 1$  yields an estimate for the constant  $C_p = C_T \kappa^{-2/3} \phi_h(\zeta) (\phi_m(\zeta) - \zeta)^{-1/3}$ . While the data in Fig. 3 cannot resolve many aspects of the regime associated with very large scales



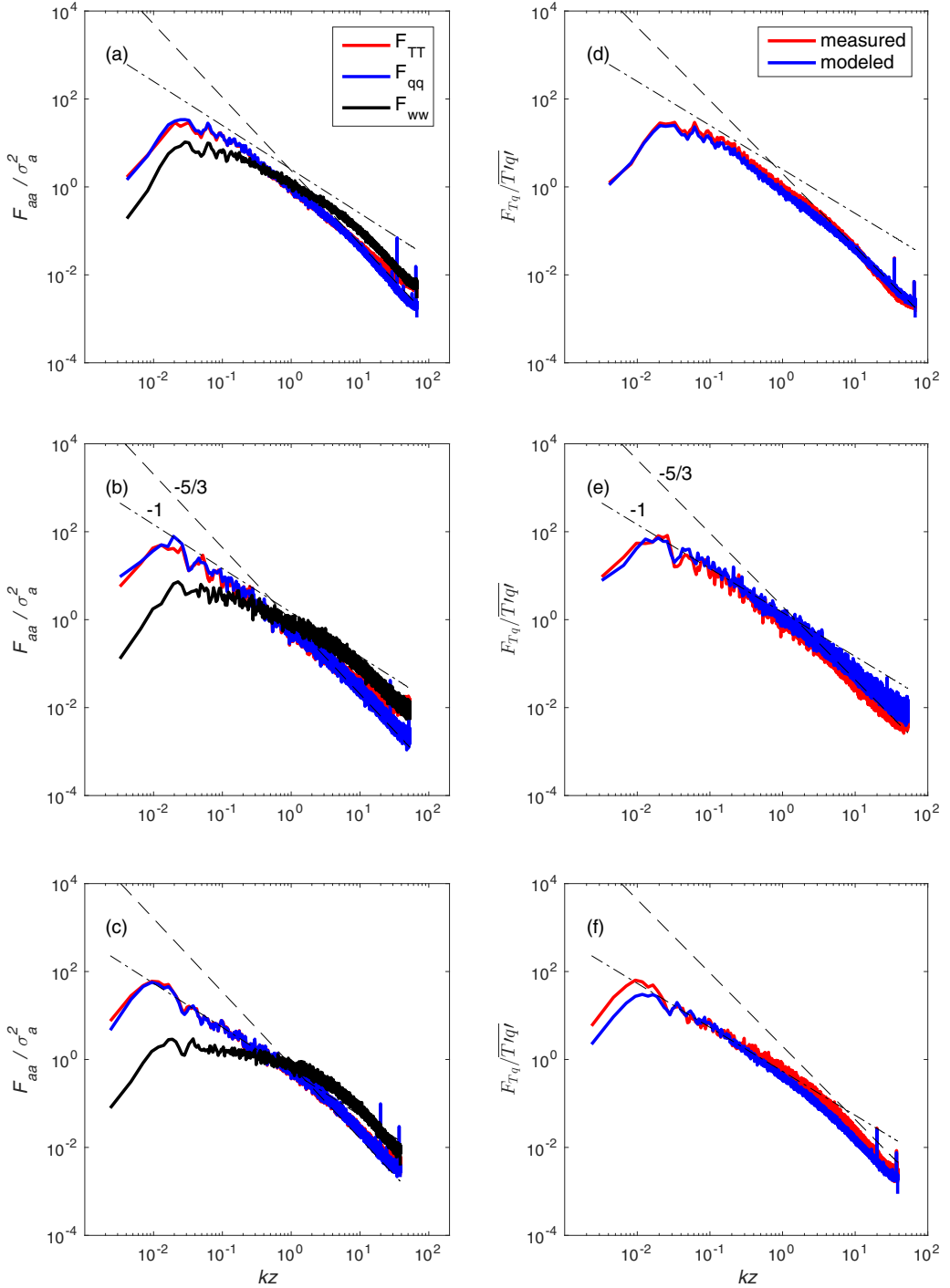


FIG. 3. Left: Variations of ensemble measured  $F_{ww}(k)/\sigma_w^2$  ( $a = w$ ),  $F_{TT}(k)/\sigma_T^2$  ( $a = T'$ ),  $F_{qq}(k)/\sigma_q^2$  ( $a = q'$ ) with normalized wave number  $kz$  for conditions  $R_{Tq} > 0.5$  (top),  $-0.5 < R_{Tq} < 0.5$  (middle), and  $R_{Tq} < -0.5$  (bottom) collected above Lake Lemman, Switzerland. For reference, the  $-1$  and  $-5/3$  power laws are shown. Right: Comparison between measured and modeled  $F_{Tq}(k)$  ( $a = T', b = q'$ ) using measured  $F_{TT}(k)/\sigma_T^2$  and  $F_{qq}(k)/\sigma_q^2$  but setting  $A_{Tq}$  (the coherence spectrum) to a constant independent of  $k$ .

( $kh_o < 1$ ), the model calculations next are based on  $F_{TT}(k) = C_p T_*^2(z/h_o)^{-1}$  being a constant for such scales extending to  $k = 0$ . The shape of  $F_{qq}(k)$  is assumed to be similar to  $F_{TT}(k)$ , which is also supported by the measurements in Fig. 3. The conditions promoting the onset of a  $-1$  power law in  $F_{TT}(k)$  for  $|\zeta| < 1$  are reviewed elsewhere [83] and are not repeated here. The scale  $h_o$  is also unambiguously interpreted as a length scale that varies in proportion to the boundary layer height.

Carrying out the integration for each region, the resulting  $I_1$  is

$$I_1 = \frac{7}{4} C_{ow} \epsilon^{1/3} z^{4/3}, \quad (36)$$

and

$$I_2 = \left[ \frac{7}{4} + \ln \left( \frac{h_o}{z} \right) \right] C_T N_T \epsilon^{-2/3} z^{4/3}. \quad (37)$$

Again, for the purposes of determining  $I_3$ , it is assumed that  $F_{Tq}(k) = A_{Tq} \sqrt{F_{TT}(k) F_{qq}(k)}$  with  $|A_{Tq}| < 1$  being constant across scales and can be evaluated from the normalizing property as

$$A_{Tq} = \frac{\overline{T'q'}}{\left[ \frac{5}{2} + \ln \left( \frac{h_o}{z} \right) \right] \sqrt{C_T C_q} \sqrt{N_T N_q} \epsilon^{-1/3} z^{2/3}}. \quad (38)$$

With this estimate for  $A_{Tq}$ ,

$$I_3 = \frac{\left[ \frac{7}{4} + \ln \left( \frac{h_o}{z} \right) \right]}{\left[ \frac{5}{2} + \ln \left( \frac{h_o}{z} \right) \right]} \overline{T'q'} \epsilon^{-1/3} z^{2/3}. \quad (39)$$

Support for such approximation to  $F_{Tq}(k)$  with  $A_{Tq}$  being held constant across scales is also shown in Fig. 3. Acceptable agreement between model calculations driven by measured  $F_{TT}(k)$  and  $F_{qq}(k)$  and measured  $F_{Tq}(k)$  is noted across all  $k$ .

Solving for  $K_T/K_q$  leads to

$$\frac{K_T}{K_q} = 1 + \Gamma_3(\zeta) \left[ R_{Tq} \frac{R_{wT}}{R_{wq}} \theta_3(\zeta) - 1 \right], \quad (40)$$

where

$$\Gamma_3(\zeta) = \left[ 1 + \frac{4}{7} \ln \left( \frac{h_o}{z} \right) \right] \frac{1 - 2\alpha_I C_T}{1 - C_I} \frac{C_T}{C_{ow}} \frac{\zeta}{\phi_m(\zeta) - \zeta}, \quad (41)$$

$$\theta_3(\zeta) = \frac{1}{\left[ \frac{5}{2} + \ln \left( \frac{h_o}{z} \right) \right]} \frac{(\kappa)^{2/3}}{C_T} \frac{[\phi_m(\zeta) - \zeta]^{1/3} [\phi_{TT}(\zeta)]^2}{\phi_h(\zeta)}. \quad (42)$$

As before,  $\Gamma_3(0) = 0$  ensures that  $K_T/K_q = 1$  for near-neutral conditions. However, dissimilarity in the shapes of  $F_{ww}(k)$  and  $F_{TT}(k)$  now results in  $\ln(h_o/z)$  impacting both  $\Gamma_3$  and  $\theta_3$  instead of  $\theta_2$  only (as for the inertial spectra case) but in opposite ways. For a given  $\zeta$ , increasing  $\ln(h_o/z)$  increases  $|\Gamma_3|$  and reduces  $\theta_3$ . As before, reductions in  $\theta_3$  reduce sensitivity of  $K_T/K_q$  on  $R_{Tq} R_{wT}/R_{wq}$ . Amplifications in  $|\Gamma_3|$  associated with increased  $h_o/z$  enhance the active role of temperature on  $K_T/K_q$ .

To explore the effects of  $z/h_o$  along with  $(R_{wT}/R_{wq})R_{Tq}$ , a comparison between models for cases 2 (inertial spectra) and 3 (realistic spectra) is featured in Fig. 4 for  $\alpha_I = 1/3$  (i.e., isotropic limit). Typical daytime  $z/h_o = 0.01$  (labeled hereafter as small  $z/h_o$ ) as well as  $z/h_o = 0.5$  (labeled hereafter as large  $z/h_o$ ) expected in stable conditions when  $h_o$  collapses are used to illustrate  $h_o$  effects above and beyond  $\zeta$ . For case 2, increasing  $z/h_o$  from 0.01 to 0.5 increases  $\theta_2$  and  $K_T/K_q (\neq 1)$  becomes sensitive to  $(R_{wT}/R_{wq})R_{Tq}$ . For the larger  $z/h_o$  in case 2,  $K_T/K_q \leq 1$  for unstable conditions even when  $(R_{wT}/R_{wq})R_{Tq} = 1$ , which cannot be reproduced by case 1 (i.e., using a single  $\tau_{\text{eff}}$ ). As expected for case 1,  $(R_{wT}/R_{wq})R_{Tq} = 1$  results in  $K_T/K_q = 1$  for

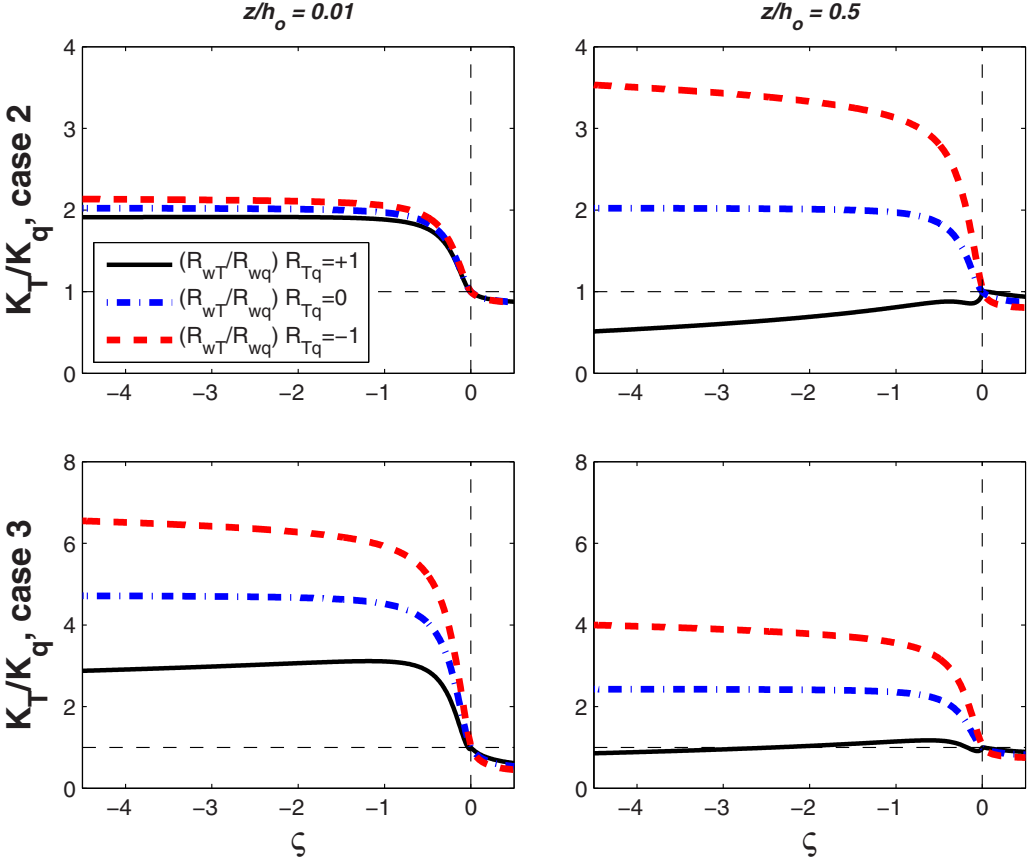


FIG. 4. Comparison between modeled  $K_T/K_q$  variations with  $\zeta$  for  $z/h_o = 0.01$  (typical for unstable atmospheric states) and  $z/h_o = 0.5$  (that can occur for stable atmospheric states) using  $\alpha_l = 1/3$ . The model runs assume  $|R_{Tq}| < 1$  but  $(R_{wT}/R_{wq})R_{Tq}$  can take on arbitrary values. The top panels are for case 2 (inertial spectra) and bottom panels are for case 3 (realistic spectra).

all stability regimes. For the smallest  $z/h_o$ , the expressions here suggest a decoupling between  $K_T/K_q$  and variations in  $(R_{wT}/R_{wq})R_{Tq}$  for case 2 (where  $\theta_2 \sim (z/h_o)^{2/3}$  becomes small) but not case 3 (where  $\theta_3 \sim [(5/2) + \log(h_o/z)]^{-1}$  remains appreciable for typical  $z/h_o$  values). Maximum deviations from unity in  $K_T/K_q$  are associated with case 3 and largest  $h_o$  (or smallest  $z/h_o$ ). For case 3, the dependency of  $K_T/K_q$  on  $(R_{wT}/R_{wq})R_{Tq}$  is far significant when compared to the previous two cases where  $h_o$  is large (or  $z/h_o$  is small). For the largest  $z/h_o$ ,  $K_T/K_q \approx 1$  when  $(R_{wT}/R_{wq})R_{Tq} \approx 1$  in case 3 as in case 1.

#### D. Comparison with experiments

The three expressions for  $K_T/K_q$  covered in cases 1 to 3 are now compared against independent estimates using data collected above a large inland water body (Ross Barnett Reservoir, Mississippi, USA) described elsewhere [69,70] in Fig. 5. The measurements include the following:  $\overline{w'q'}$ ,  $\overline{w'T'}$ ,  $\overline{w'w'}$ ,  $\overline{q'q'}$ ,  $\overline{T'T'}$ ,  $\overline{T'q'}$ ,  $\overline{w'u'}$  at 10-Hz sampling frequency with averaging conducted over 30-min intervals, as well as  $\overline{T_s}$ ,  $\overline{T}$ , and  $\overline{q}$  at  $z = 4$  m. The  $h_o$  was not measured in the experiment but was estimated using the expression  $h_o = C_z u_* / f_{\text{cor}}$ , where  $C_z = 0.3$  is a similarity constant inferred for near-neutral conditions, and  $f_{\text{cor}} = 1 \times 10^{-4} \text{ rad s}^{-1}$  is the Coriolis frequency [84]. This estimate likely under-estimates  $h_o$  in convective conditions and overestimates  $h_o$  in stable

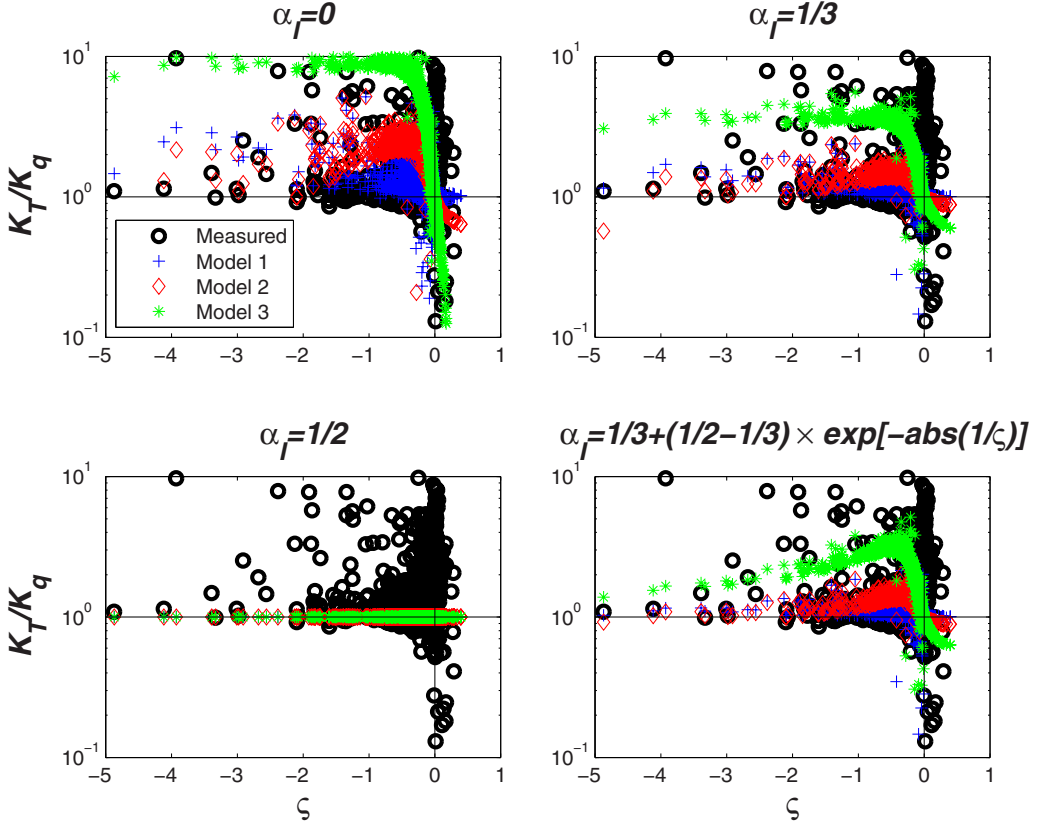


FIG. 5. Comparison between modeled  $K_T/K_q$  with  $\zeta$  using estimated  $h_o$  [84] and measured  $(R_{wT}/R_{wq})R_{Tq}$  for the Ross Barnett Reservoir (Mississippi, USA) for various  $\alpha_I$  to illustrate model sensitivity. Models 1, 2, and 3 correspond to the final formulation in cases 1, 2, and 3, respectively, but using measured  $R_{Tq}R_{wT}/R_{wq}$  shown in Fig. 2.

conditions. Given the uncertainty in  $\alpha_I$ , the comparison in Fig. 5 is conducted for  $\alpha_I = 0$ ,  $\alpha_I = 1/3$  (isotropic case),  $\alpha_I = 1/2$  (suggested for convective conditions from LES studies), and an ad hoc stability dependent  $\alpha_I = 1/3 + (1/2 - 1/3) \times \exp[-|\zeta^{-1}|]$ . This functional dependency ensures that  $\alpha_I \approx 1/3$  for near-neutral conditions ( $|\zeta| \approx 0$ ) and  $\alpha_I \approx 1/2$  for near-convective conditions ( $-\zeta \rightarrow \infty$ ). When  $\alpha_I = 1/3$ , cases 1 and 2 reasonably agree with the independent estimates in Fig. 5 that  $K_T/K_q > 1$  for moderate to strongly unstable conditions. Case 3 captures the rapid rise in  $K_T/K_q$  as atmospheric stability regime transitions from its near-neutral to mildly unstable state (especially for  $\alpha_I = 0$ ), but overestimates  $K_T/K_q$ . The overestimation is not surprising as the spectral shapes assumed for case 3 are appropriate for near-neutral and mildly unstable flow whereas air temperature and vertical spectra tend to follow an approximate  $-5/3$  scaling for strongly unstable conditions (i.e., resembling the analysis in case 2). As expected, reducing  $\alpha_I$  from its  $1/2$  value increases modeled  $K_T/K_q$ , especially for the formulation in case 3. The stability-dependent  $\alpha_I$  prescribed here results in a nonmonotonic shape for modeled  $K_T/K_q$ , especially for the formulations covered in cases 2 and 3. Hence, it is evident here that  $K_T/K_q$  variations are sensitive to deviations in  $\alpha_I$  from  $1/2$  though in the absence of any other guidance, setting  $\alpha_I = 1/3$  appears plausible for cases 1 and 2 for unstable conditions, and case 3 for near-neutral to transitioning to unstable conditions.

### III. CONCLUSION

The three expressions for  $K_T/K_q$  derived for the nontrivial case  $|R_{Tq}| < 1$  but arbitrary  $R_{Tq}R_{wT}/R_{wq}$  are the sought results. The  $|R_{Tq}| < 1$  in the atmosphere is guaranteed by the near anticorrelation at the top of the atmospheric boundary layer. Attainment of  $K_T/K_q \approx 1$  is due to a competition between the active role of temperature encoded here in  $\Gamma_1$ ,  $\Gamma_2$ , and  $\Gamma_3$  and dissimilarity in heat and water vapor transport as captured by the term  $(R_{wT}/R_{wq})R_{Tq}$ . A  $K_T/K_q = 1$  emerges from all cases when (i)  $|\zeta| \rightarrow 0$  no matter what  $h_o/z$  or  $(R_{wT}/R_{wq})R_{Tq}$  values they take. Also,  $K_T/K_q = 1$  for any  $|\zeta|$ ,  $z/h_o < 1$  or  $(R_{wT}/R_{wq})R_{Tq}$  if  $\alpha_I$  is increased to  $1/2$  (suggested by some LES studies for convective boundary layers). In other cases,  $K_T/K_q \neq 1$  even when  $(R_{wT}/R_{wq})R_{Tq} = 1$  (provided  $R_{Tq} < 1$ ) in cases 2 and 3, but not in case 1.

In summary, the work here (cases 2 and 3) demonstrated that when  $|R_{Tq}| < 1$ , deviations in  $K_T/K_q$  from unity depend on  $z/L$  and  $z/h_o$  as well as the dissimilarity measure  $(R_{wT}/R_{wq})R_{Tq}$ . The sensitivity of  $K_T/K_q$  to  $z/L$ ,  $z/h_o$  and  $(R_{wT}/R_{wq})R_{Tq}$  is also influenced by the spectral shapes of vertical velocity, air temperature, and water vapor. Such sensitivity cannot be inferred from classical higher-order closure schemes that utilize a master length or time scale.

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