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## **Parameters for the Collapse of Turbulence in the Stratified Plane Couette Flow**

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#### ABSTRACT

We perform direct numerical simulation of the Couette flow as a model for the stable boundary layer. The flow evolution is investigated for combinations of the (bulk) Reynolds number and the imposed surface buoyancy flux. First, we establish what the similarities and differences are between applying a fixed buoyancy difference (Dirichlet) and a fixed buoyancy flux (Neumann) as boundary conditions. Moreover, two distinct parameters were recently proposed for the turbulent-to-laminar transition: the Reynolds number based on the Obukhov length and the ''shear capacity,'' a velocity-scale ratio based on the buoyancy flux maximum. We study how these parameters relate to each other and to the atmospheric boundary layer. The results show that in a weakly stratified equilibrium state, the flow statistics are virtually the same between the different types of boundary conditions. However, at stronger stratification and, more generally, in nonequilibrium conditions, the flow statistics do depend on the type of boundary condition imposed. In the case of Neumann boundary conditions, a clear sensitivity to the initial stratification strength is observed because of the existence of multiple equilibriums, while for Dirichlet boundary conditions, only one statistically steady turbulent equilibrium exists for a particular set of boundary conditions. As in previous studies, we find that when the imposed surface flux is larger than the maximum buoyancy flux, no turbulent steady state occurs. Analytical investigation and simulation data indicate that this maximum buoyancy flux converges for increasing Reynolds numbers, which suggests a possible extrapolation to the atmospheric case.

#### 1. Introduction

To reduce the complexity of studying the stably stratified atmospheric boundary layer (SBL), we often resort to idealized, conceptual models (André [and Mahrt](#page-19-0) [1982;](#page-19-0) [McNider et al. 1995](#page-20-0); [Wilson and Venayagamoorthy](#page-21-0) [2015;](#page-21-0) [van Heerwaarden and Mellado 2016](#page-21-1); [van de Wiel](#page-21-2) [et al. 2017;](#page-21-2) [Fedorovich et al. 2017](#page-20-1)). A particularly useful tool with respect to idealized flow configurations is direct numerical simulation (DNS; [Moin and Mahesh](#page-20-2) [1998;](#page-20-2) [Marlatt et al. 2012](#page-20-3); [Fritts et al. 2016\)](#page-20-4) since it does not require any parameterization of turbulence. Among other limitations, a major drawback of employing DNS is that it cannot resolve flows at atmospheric Reynolds numbers (the scale separation between the largest and smallest scales of turbulence, defined in [section 2](#page-3-0)). As such, it is not always clear how the results extend to the atmospheric case. In this study, we aim to understand how previous advances on the collapse of turbulence based on canonical flow configurations relate to each other. Additionally, we discuss their applicability to the real SBL.

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Traditionally, the transition in the SBL was associated with a characteristic value of the Obukhov parameter  $z/L$  (with z the height above the surface and L the Obukhov length; [Monin 1970\)](#page-20-5) or a Richardson number. Recently, doubt was cast on the suitability of these parameters to mark a transition of the global character of the SBL from weakly stable (WSBL) to very stable (VSBL) ([Grachev et al. 2013](#page-20-6); [van Hooijdonk et al. 2015;](#page-21-3) [Monahan et al. 2015](#page-20-7)]). As an alternative, [van Hooijdonk](#page-21-3) [et al. \(2015\)](#page-21-3) used the existence of a maximum in the sensible heat flux transport in the SBL [\(Taylor 1971;](#page-21-4) [Malhi 1995;](#page-20-8) [van de Wiel et al. 2007](#page-21-5)) to introduce a new dimensionless ratio coined the ''shear capacity.'' This ratio indicates whether or not the wind speed is strong enough to generate a turbulent heat flux that compensates the radiative energy loss of low-heat-capacity surfaces. Using field observations, [van Hooijdonk et al.](#page-21-3) [\(2015\)](#page-21-3) and [Monahan et al. \(2015\)](#page-20-7) showed that this parameter broadly separates the VSBL from the WSBL. In a DNS of a Couette flow, [van Hooijdonk et al. \(2017b\)](#page-21-6) showed that turbulence collapses when this ratio is less than a critical value.

Several recent studies showed interesting results using DNS of boundary layer flows over a smooth wall with respect to the transition from a turbulent flow to an intermittent or laminar flow. It appears that this transition occurs when stratification suppresses the near-wall generation of turbulence, which was characterized by the so-called Obukhov–Reynolds number [\(Flores and](#page-20-9) [Riley 2011](#page-20-9)). This parameter indicates the ratio between the Obukhov length  $L$  ([Monin 1970\)](#page-20-5) and the smallest turbulent length scale, the wall unit  $\nu/u_\tau$  (e.g., [Kim et al.](#page-20-10) [1987\)](#page-20-10). Several studies show that for a large range of Reynolds numbers  $[O(10^3)-O(10^5)]$  and for different configurations the transition to intermittent or laminar occurs when this ratio is  $O(100)$  ([Flores and Riley 2011;](#page-20-9) [Deusebio et al. 2015;](#page-20-11) [Ansorge and Mellado 2016;](#page-19-1) [Zhou](#page-21-7) [et al. 2017\)](#page-21-7). This transition was explicitly associated with the transition from a WSBL to a VSBL as defined by [Mahrt et al. \(1998\)](#page-20-12), although it is unclear how this transition parameter translates to rough surfaces. Moreover, a truly laminar flow is unlikely to occur in the real SBL, as indicated by observations ([Mauritsen et al.](#page-20-13) [2007\)](#page-20-13) and the occurrence of intermittency in numerical simulations at supercritical stability ([Ansorge and](#page-19-2) [Mellado 2014](#page-19-2)), that is, where traditional stability analysis predicts laminarization.

Both the shear capacity and the Obukhov–Reynolds number indicate a transition in strongly stratified idealized flows. One possibility is that the two parameters are essentially the same. However, the shear capacity is expressed using bulk variables (wind speed, height), while the Obukhov–Reynolds number is expressed in wall variables (friction velocity, surface heat flux). Therefore, it is unlikely that both parameters have the same physical meaning. Consequently, we may ask the following questions: How do these parameters relate to each other? What is their respective physical relevance? And what is their relevance for the SBL?

To answer these questions, we perform DNS of the Couette flow with a fixed heat (or, more generally, buoyancy) flux (Neumann) boundary conditions (BCs) imposed at the top and bottom walls. We opt for DNS instead of large-eddy simulation (LES; e.g., as in [Armenio and Sarkar 2002\)](#page-19-3) since the closure paradigms of LES are violated in strongly stratified, intermittent flows. We investigate the flow at several combinations of the (bulk) Reynolds number and the shear capacity, which are the external parameters for this configuration. Thereby, this investigation directly extends the results of [van Hooijdonk et al. \(2017b\)](#page-21-6). The results of these simulations are then discussed in relation to previous studies of related configurations using DNS (with cooling turned on instantly at  $t = 0$ ), such as the Ekman flow ([Ansorge and Mellado 2016](#page-19-1); [Gohari and Sarkar 2017](#page-20-14)), the plane channel flow [\(Flores and Riley 2011;](#page-20-9) [Garc](#page-20-15)ía-[Villalba and del](#page-20-15) Álamo 2011), and the Couette flow with a fixed bulk temperature difference ([Deusebio](#page-20-11) [et al. 2015\)](#page-20-11).

Between these configurations, there is a clear hierarchy, with the Ekman flow being the most realistic, but also the most complex, configuration. Here, we opt for investigating the Couette flow for three reasons: First, symmetry of the problem allows us to combine the DNS results with analytical considerations. Second, as argued in [van de Wiel et al. \(2012a\)](#page-21-8) and [van Hooijdonk et al.](#page-21-6) [\(2017b\)](#page-21-6), this configuration captures several essential features of the real SBL in the first few hours after sunset, particularly in relation to the WSBL–VSBL transition. Third, the collapse of turbulence (i.e., laminarization that is permanent or local in time and/or space) due to a stable density gradient appears to be controlled by the same mechanism in different wallbounded flow configurations ([Scotti and White 2016;](#page-21-9) [Zhou et al. 2017](#page-21-7)).

Generality of the collapse mechanism also exists between different temperature BCs [\(Flores and Riley](#page-20-9) [2011;](#page-20-9) [Mellado 2012](#page-20-16); [Deusebio et al. 2015\)](#page-20-11), but there is no clear hierarchy in terms of realism between imposing a constant heat flux or isothermal walls. The most realistic choice would evidently be the inclusion of a soil model (e.g., as in [Smirnova et al. 1997;](#page-21-10) [Steeneveld et al. 2006](#page-21-11)). However, this requires additional model choices and may not be feasible computationally. Therefore, idealized surfaces are typically used in conceptual studies [\(Garg et al.](#page-20-17) [2000](#page-20-17); [Ansorge and Mellado 2014](#page-19-2)). Since the applicability

of different temperature BCs has been debated in several papers [\(Basu et al. 2008](#page-19-4); [Gibbs et al. 2015;](#page-20-18) [van de](#page-21-2) [Wiel et al. 2017](#page-21-2)), a particular question is, What is the relative impact of choosing imposed fluxes (Neumann) or isothermal walls (Dirichlet) as BCs for buoyancy? The advantage of the latter is that it allows for more control over the stratification strength, since the bulk stratification does not dynamically interact with the flow. But in reality, dynamical interactions between the bulk buoyancy gradient and turbulent mixing may be very important, for example, for predictions of the nighttime surface temperature ([Fernando and Weil 2010;](#page-20-19) [Holtslag et al. 2013](#page-20-20)).

To study the impact of the temperature BCs, we also apply DNS. Unlike one-dimensional eddy viscosity [Reynolds-averaged Navier–Stokes (RANS)] models of similar systems ([van de Wiel et al. 2007;](#page-21-5) [Holdsworth](#page-20-21) [et al. 2016;](#page-20-21) [van de Wiel et al. 2017](#page-21-2)), DNS does not rely on the assumption that the flow is horizontally homogeneous or that turbulent fluxes are in instantaneous equilibrium with the mean flow. Both assumptions become invalid for a fast-evolving strongly stratified flow. As such, a DNS may be used to reevaluate RANS-based predictions of the dynamical behavior.

In summary, this paper aims to identify 1) how the critical value of the shear capacity ([van Hooijdonk et al.](#page-21-6) [2017b\)](#page-21-6) relates to the transition marked by the Obukhov– Reynolds number and 2) what the differences and similarities are, both in terms of temporal evolution and the statistically steady state, between applying a fixed flux (Neumann) or a fixed difference (Dirichlet) as temperature BC for the Couette flow.

Following the presentation of specific methods, parameters, and simulation strategy in [section 2,](#page-3-0) we extend the findings of [van Hooijdonk et al. \(2017b\)](#page-21-6) by discussion of the flow characteristics as function of the shear capacity [\(section 3a](#page-5-0)). Boundary conditions (flux driven or isothermal) are analyzed by comparison of the steady-state statistics as well as the dynamical behavior [\(section 3b](#page-8-0)). For the Dirichlet cases, we use the DNS of [Deusebio et al.](#page-20-11)  $(2015)$  for interpretation, and a quantitative comparison is made with additional simulations. We further investigate the relation between the critical value of the shear capacity, which is associated with maximization of the turbulent buoyancy flux ([van Hooijdonk et al. 2015,](#page-21-3) [2017b](#page-21-6)), with the Reynolds number ([section 3c\)](#page-10-0) as well as the Obukhov–Reynolds number ([section 3d](#page-11-0)). The gradient Richardson number at the centerline of the flow is shown to be associated with a maximum buoyancy flux in [section](#page-13-0) [3e,](#page-13-0) while the bulk Richardson number does not seem to govern the collapse adequately. This presentation is finalized by the discussion ([section 4\)](#page-15-0) and summarizing conclusions ([section 5\)](#page-16-0).

#### <span id="page-3-0"></span>2. Theory and methods

#### a. Model setup and dimensionless numbers

The Couette flow consists of a horizontally infinite domain (mimicked by periodic BCs), which is vertically symmetric around the centerline at  $z = h$ , and it is vertically bounded by the walls at  $z = 0$  and  $z = 2h$ . These walls are moving in opposite directions with velocity  $\pm U_0$ . The horizontal motion of the walls generates a shear layer in between the walls. As argued in [van de](#page-21-12) [Wiel et al. \(2012b\)](#page-21-12), around sunset, a height exists around which the wind velocity is close to constant. We consider the bottom half of the Couette flow a model for the SBL during this period [e.g., see the sketches in Fig. 1 of [Zhou](#page-21-7) [et al. \(2017\)\]](#page-21-7). Furthermore, a constant wall flux is being used as a model for the relatively constant net radiative energy loss of an isolating surface under clear-sky conditions in relatively dry environments. On Antarctica, such conditions are approximated quite closely ([Vignon](#page-21-13) [et al. 2017\)](#page-21-13), while in general, this approximation is rather crude.

<span id="page-3-1"></span>For this setup, the governing flow equations for an incompressible fluid under the Boussinesq approximation are

$$
\frac{\partial u_i}{\partial x_i} = 0,\t\t(1a)
$$

$$
\frac{\partial u_i}{\partial t} = -u_j \frac{\partial u_i}{\partial x_j} - \frac{1}{\rho_0} \frac{\partial p}{\partial x_i} - b \delta_{i3} + \nu \frac{\partial^2 u_i}{\partial x_j^2},\tag{1b}
$$

<span id="page-3-2"></span>
$$
\frac{\partial b}{\partial t} = -u_j \frac{\partial b}{\partial x_j} + \kappa_b \frac{\partial^2 b}{\partial x_j^2},\tag{1c}
$$

for conservation of mass, momentum, and heat, respectively (Einstein summation convention applies). In these equations,  $u_i$  represents the velocity components  ${u_1 = u, u_2 = v, u_3 = w}$  of a fluid parcel at time t and position  $\{x_1 = x, x_2 = y, x_3 = z\}$ ,  $\delta_{ij}$  is the Kronecker delta ( $\delta_{ij}$  = 1 when *i* = *j* and 0 otherwise), *p* is the pressure,  $\rho_0$  the reference density,  $\nu$  is the kinematic viscosity, and  $\kappa_b$  is the molecular diffusion of buoyancy. For generality, we define the buoyancy  $b = gT/T_0$ , with T the temperature deviation with respect to an arbitrary reference temperature  $T_0 \gg T$  and g the acceleration by gravity.

For this setup we define the (bulk) Reynolds number as  $\text{Re} = U_0 h / \nu$ , which varies between 1000 and 6200, at least three to four orders of magnitude lower than for the real SBL. The molecular Prandtl number  $(Pr = \nu/\kappa_b)$  is kept constant at 1 for simplicity. Recent findings by [Zhou et al. \(2017\)](#page-21-7) indeed suggested that there is only a very minor impact of varying between  $Pr = 1$  and  $Pr = 0.7$  (the value for air). The definition of the external stratification parameter depends on the buoyancy BCs.

For velocity, no-slip BCs are imposed; that is,  $u = \pm U_0$ and  $v = w = 0$  at the walls. Horizontally, a periodic domain is being used. For buoyancy, we apply Neumann (flux) BCs in most cases; that is,

$$
\partial_z b_{\text{wall}} = q_w / \kappa_b, \qquad (2)
$$

with  $-q_w$  the imposed buoyancy flux through the walls. The external control parameter is then the shear capacity of the Couette flow [\(van Hooijdonk et al. 2017b](#page-21-6)), which is defined as

$$
SC_C = U_0 / (hq_w)^{1/3}.
$$
 (3)

Physically,  $SC_C$  represents a ratio of velocity scales:  $U_0$  is the wall velocity, and  $(hq_w)^{1/3}$  is proportional to the velocity at the maximum total (diffusive plus turbulent) buoyancy flux  $\phi_{b,\text{max}}$  equals  $q_w$ , which occurs at value  $SC_C = SC_C^{crit}$ . Thus,  $SC_C^{crit}$  indicates whether or not the turbulent flow can sustain the buoyancy flux needed to match the BC. In the Couette flow,  $SC_C$  provides a definite answer (at least for a given Re; see [van](#page-21-6) [Hooijdonk et al. 2017b\)](#page-21-6) about the final state of the flow being turbulent or laminar. For the plane channel flow, this may be different. In that configuration, turbulence may collapse temporarily when  $q_w$  is too large [\(Flores](#page-20-9) [and Riley 2011\)](#page-20-9). Subsequently, turbulence recovers because of reacceleration of the flow [\(Businger 1973;](#page-19-5) [Donda et al. 2015](#page-20-22)). [Donda et al. \(2015\)](#page-20-22) showed that when a different initial velocity profile (i.e., one for which shear is initially larger than in a logarithmic profile) was used, the flow may remain turbulent at all times.

The bulk Richardson number  $\mathrm{Ri}_b$  is defined as

$$
\text{Ri}_b = \frac{h\Delta b}{U_0^2},\tag{4}
$$

with  $\Delta b = 0.5[b(z = 2h) - b(z = 0)].$  In the flux-driven case (with  $SC<sub>C</sub>$  as an external parameter),  $Ri<sub>b</sub>$  is an internal parameter representing the bulk stratification. In case Dirichlet BCs for buoyancy are being applied, it is  $\Delta b = B_0$ , with  $\pm B_0$  the imposed buoyancy at the walls.

While Re is the external parameter setting the scale separation, it is not the exact turbulence scale separation of the flow. The latter is related to the—a priori unknown—wall friction. The actual scale separation between the domain-scale  $h$  and the smallest-scale  $\nu/u_{\tau}$  is described by the friction Reynolds number  $\text{Re}_{\tau} = u_{\tau} h / \nu$ , with  $u_{\tau}^2 = \nu [\partial_z u] (z = 0)$ . This parameter characterizes the near-wall behavior of the flow. Taking into account the limiting effect of stability on the largest scales, [Flores and Riley \(2011\)](#page-20-9) introduced an <span id="page-4-1"></span>additional scale separation, the Obukhov–Reynolds number, defined as

$$
\text{Re}_L = \frac{L u_\tau}{\nu},\tag{5}
$$

with  $L = u_\tau^3 / (\kappa q_w)$  the Obukhov length and  $\kappa$  the von Kármán constant. The Obukhov length is interpreted as the height at which buoyancy becomes more limiting for turbulence than the wall distance. For  $L \le O(h)$ , the Obukhov–Reynolds number indicates the ratio of the size of the largest turbulent motions of  $O(L)$  compared to the smallest turbulent motion of  $O(\nu/u_\tau)$ . [Flores and](#page-20-9) [Riley \(2011\)](#page-20-9) suggested that turbulence cannot survive when this ratio is less than  $O(100)$ . The scale separation  $Re<sub>L</sub>$  is based on similar arguments as the buoyancy Reynolds number [\(Smyth and Moum 2000](#page-21-14); [Billant and](#page-19-6) [Chomaz 2001;](#page-19-6) [Brethouwer et al. 2007](#page-19-7)), defined as

$$
\text{Re}_b = \left(\frac{l_0}{\eta}\right)^{4/3} = \frac{\varepsilon_{\text{tke}}}{\nu N^2},\tag{6}
$$

in which  $l<sub>O</sub>$ , the Ozmidov scale, defines the length scale below which turbulence is assumed to be isotropic;  $\eta$  is the Kolmogorov length scale;  $\varepsilon_{\text{tke}}$  is the dissipation of the turbulent kinetic energy (TKE); and  $N = \sqrt{\partial_z b}$ is the Brunt–Väisälä frequency (also called buoyancy frequency). It was suggested that this parameter provides a better characterization of strongly stratified flows than a Richardson number (e.g., [Shih et al. 2005;](#page-21-15) [Bartello and Tobias 2013\)](#page-19-8). The parameters  $Re<sub>L</sub>$  and  $Re<sub>b</sub>$  are related as

$$
\text{Re}_b \simeq \kappa \text{Re}_L,\tag{7}
$$

<span id="page-4-0"></span>by assuming the scaling relations  $\varepsilon_{\text{tke}} \sim u_{\tau}^3/l$  and  $N^2 \sim$  $q_w/(u_\tau l)$ . In this relation, l is the mixing length (assumed equal for momentum and buoyancy). The DNS results by [Zhou et al. \(2017\)](#page-21-7) show good agreement with [\(7\)](#page-4-0) for a wide range of Re, Pr, and  $\text{Ri}_b$ . Since both  $\varepsilon_{\text{tke}}$  and N are height dependent, the numerical values of  $Re<sub>b</sub>$ may depend on the averaging volume. Conversely,  $Re<sub>L</sub>$ takes a single value, since it is defined based on wall variables only. Therefore,  $Re<sub>L</sub>$  is likely more relevant for characterizing the state of the SBL, and hence, we focus our discussion on this parameter.

### b. Numerical method

Equations  $(1a)$ – $(1c)$  are solved using the DNS algorithm of [van Heerwaarden et al. \(2017](#page-21-16); [https://github.](https://github.com/microhh/microhh) [com/microhh/microhh\)](https://github.com/microhh/microhh). The algorithm is used with a fractional-step [\(Kim and Moin 1985](#page-20-23)) third-order Runge– Kutta scheme for time integration and a CFL number of 1. The spatial discretization is of second order, and it is based on finite differences, with uniformly distributed grid points. The code also allows for fourth-order accuracy, but since no significant differences were observed when, for example, evaluating the dissipation profiles, the second-order spatial discretization is used to limit computational cost.

Profiles of statistical quantities (e.g., budget terms of the Reynolds stresses) were stored at each time unit  $h/U_0$ . To this end, the flow variables are Reynolds decomposed into horizontally averaged fields  $U_i = \langle u_i \rangle$ ,  $B = \langle b \rangle$ (where  $\langle \cdot \rangle$  indicates averaging in the horizontal plane) and fluctuating fields  $u'_i = u_i - U_i$ ,  $b' = b - B$ . Unless stated otherwise, these quantities are presented in inertial units, that is, normalized using  $U_0$  and h.

The resolution is chosen such that under neutral stratification it is in the range  $2.5-5.4\nu/u_t$  horizontally and 0.7–1.4 $\nu/u_t$  vertically. A list of the resolution for each simulation is presented in [appendix A](#page-17-0) [\(Table A1\)](#page-18-0). We verified that the budget terms of the TKE agree very closely between different Reynolds numbers and with previous numerical results under neutrally stratified conditions (appendix  $B$ ). Moreover, we verified the height independence of the total fluxes of momentum and buoyancy.

#### c. Case setup

A specific goal is to determine the critical value of  $SC_C$ below which turbulence cannot be sustained at each Re. We investigate the flow evolution for decreasing values of  $SC_C$  at six values of Re. For each Re, the Couette flow is initialized with a randomly perturbed logarithmic profile. Equations [\(1\)](#page-3-2) are then solved for  $250-300h/U_0$ until a turbulent, statistically steady state is obtained. The final state of the neutral initialization is then used as the initial condition for the stratified cases with the corresponding Reynolds number. When  $SC_C \approx 22-24$ , a significantly longer time was required to reach a steady state. Therefore, to limit computational cost, two cases are started from fully turbulent fields instead of starting from the neutrally stratified initial state (see [Table 1](#page-6-0)).

When possible, the time-averaged steady-state values of  $\text{Re}_{\tau}$ ,  $\text{Re}_{L}$ , and  $\text{Ri}_{h}$  were obtained. These values are also listed in [Table 1](#page-6-0) for comparison. The relative standard deviation of each quantity is approximately 1% or less (measured by the standard deviation during the averaging period). If a simulation does not acquire a statistically steady state within the simulated time (marked with an asterisk in [Table 1\)](#page-6-0), the final value of these dimensionless ratios is listed.

To investigate the effect of the initial and the BCs, additional simulations are performed [\(Table 2\)](#page-7-0). To compare the steady-state statistics, the steady-state  $\text{Ri}_b$ is measured for several cases in which Neumann BCs are used. This value for  $\mathrm{Ri}_b$  is then used as a control parameter in a new simulation (labeled RxxRxxx), in which Dirichlet BCs are used. The difference between applying Dirichlet or Neumann BCs is the quantities that are fixed at the top and bottom boundary, summarized as follows:

- Dirichlet BC:  $b_{\text{wall}}$  fixed,  $\partial_z b_{\text{wall}}$  free;
- Neumann BC:  $b_{\text{wall}}$  free,  $\partial_z b_{\text{wall}}$  fixed.

Another set of simulations is initialized with a strongly stratified state of the flow (labeled RxxVSxxx). For these cases, Neumann BCs are imposed such that  $SC_C > SC_C^{\text{crit}}$ , as listed in [Table 2,](#page-7-0) to investigate the evolution for different initial conditions.

#### 3. Results

#### <span id="page-5-0"></span>a. Flow characteristics versus the shear capacity

In this section, we investigate the evolution of the flow at different  $SC<sub>C</sub>$ , as well as the steady state of the flow when  $SC_C < SC_C^{crit}$ . Particularly, we investigate if the results at  $Re = 3500$  are consistent with previous studies. A comparison between different Re is made in subsequent sections.

[Figure 1a](#page-7-1) shows the velocity profile for each value of  $SC_C$  at Re = 3500. For  $SC_C \ge 23.7$  (based on the present simulations), the profiles correspond to a statistically steady state. For these cases, the Obukhov length is still larger than the domain half height (e.g., at  $SC_C = 23.7$ ,  $h/L \approx 0.32$ ), which indicates a weak influence of the density gradient. When  $SC_C < 23.7$ , the flow is not in a steady state at the end of the simulation. For these cases, a tendency toward a linear profile (the laminar steady state) is observed, with the exception of case R35S231 (i.e.,  $Re = 3500$ ,  $SC_C = 23.1$ ), for which it is unclear if a turbulent steady state can be maintained. In agreement with Deusebio et al.  $(2015; \text{ using } Pr = 0.7)$ , we find that the buoyancy profiles ([Fig. 1b](#page-7-1)) are similar in shape to the velocity profile at a Prandtl number of order unity.

[Zhou et al. \(2017\)](#page-21-7) suggested that the gradient Richardson number  $\text{Ri} = \langle \partial_z b \rangle / [\langle \partial_z u \rangle]^2$  cannot exceed<br>0.2 in a turbulent Couette flow, Indeed, we find that Bi 0.2 in a turbulent Couette flow. Indeed, we find that Ri nowhere exceeds  $0.195$  for  $Re = 6200$  (with even lower values for lower Re). Although this corresponds closely to the limit predicted by [Zhou et al. \(2017\)](#page-21-7), we cannot exclude the possibility that Ri exceeds 0.2 at even larger Reynolds numbers based on the present results.

Within the atmospheric context, it is well known that turbulence may exist at  $\text{Ri} \gg 0.2$  (and also  $h/L \gg 0.32$ ).<br>As such caution needs to be taken when extrapolating As such, caution needs to be taken when extrapolating current results to the real atmosphere. In the atmospheric

<span id="page-6-0"></span>



TABLE 1. Overview of all simulations with Neumann BCs. Single asterisks indicate that no steady state was reached during the simulation. The double asterisks indicate initialization

<span id="page-7-0"></span>

TABLE 2. Overview of additionally performed runs with Dirichlet BCs or different initial conditions. The columns are as in [Table](#page-6-0) 1. For runs that are labeled Rxx

<span id="page-7-1"></span>

FIG. 1. (a) Dimensionless velocity and (b) buoyancy profiles between  $z = 0$  and  $z = h$  for all SC<sub>C</sub> at Re = 3500. Each symbol corresponds to a value of SC<sub>C</sub>:  $\infty$  ( $\Box$ ), 31.7 ( $\diamond$ ), 27.1 ( $\nabla$ ), 23.7 (+), 23.1 ( $\times$ ), 22.5 ( $\times$ ), 22.0 ( $\triangle$ ), and 21.5 ( $\star$ ).

VSBL, Ri values may greatly exceed the value of 0.2 [\(Mauritsen et al. 2007](#page-20-13); [Sun et al. 2015](#page-21-17)). In particular, processes like clear-air radiative cooling and advection [\(Derbyshire 1999\)](#page-19-9) and subsidence ([Vignon et al. 2017](#page-21-13)) may result in  $\mathrm{Ri} > 0.2$ . When extrapolating the present results, one should take into account that these processes are not within our scope.

The bulk Richardson number evidently increases with decreasing SC<sub>C</sub> [\(Fig. 2a](#page-8-1)). Once  $SC_C < SC_C^{crit}$  is in the range of 23.1–23.7, stratification grows significantly in time, and no statistically steady state is reached within the simulated time. The value of  $\mathrm{Ri}_b$  that corresponds to a laminar steady state (linear profiles) is given by

$$
Ri_b^{\text{lam}} = SC_C^{-3}RePr
$$
 (8)

(e.g.,  $\text{Ri}_b^{\text{lam}} = 0.35$  for case R35S215). No case was simulated long enough such that values of  $\text{Ri}_b \gtrsim \text{Ri}_b^{\text{lam}}/2$ were found. However, the simulation length of some cases was sufficient to observe purely viscous buoyancy transport (albeit not in steady state), that is, coinciding with the prediction  $\phi_b h / U_0^3 = Ri_b / Re$  (not shown), where  $\phi_b$  is the total buoyancy flux.

All cases resulting in a turbulent steady state  $(\text{SC}_C > \text{SC}_C^{\text{crit}})$  have values of  $\text{Re}_L \ge 500$  [\(Fig. 2b](#page-8-1); [Table 1](#page-6-0)). Conversely, turbulence collapses once  $SC_C < SC_C^{crit}$ , as indicated by a runaway decrease of  $Re<sub>L</sub>$ . The buoyancy

Rxxx (based on the

<span id="page-8-1"></span>

FIG. 2. Evolution of (a)  $\text{Ri}_b$  and (b)  $\text{Re}_b$  for all  $\text{SC}_c$  at  $\text{Re} = 3500$ . Symbols are as in [Fig. 1](#page-7-1). Dashed horizontal lines in (b) indicate  $Re_L = 200$  and  $Re_L = 500$ .

variance  $\langle b^2 \rangle$  maximizes around Re<sub>L</sub>  $\approx$  150 ([Fig. 3a](#page-8-2)) while the buoyancy gradient  $\langle \partial_z b \rangle$  keeps increasing for higher Re<sub>L</sub>. Such a decrease of  $\langle b^2 \rangle$  requires a decrease of  $\langle b'w' \rangle_{z=h}$ , overcompensating for the growth in  $\langle \partial_z b \rangle$ <br>with Be. Indeed as observed in Fig. 3b, the buoyancy with  $Re<sub>L</sub>$ . Indeed, as observed in [Fig. 3b,](#page-8-2) the buoyancy flux is maximized already before the collapse occurs, that is, when  $Re<sub>L</sub>$  is still in the range of 270–350. The sharp decrease of the buoyancy flux around  $Re<sub>L</sub> \approx 150$ causing a decrease of  $\langle b^2 \rangle$  (despite increasing stratification) hence results from a simultaneous breakdown of both  $\langle w^2 \rangle$  and  $\langle b'w' \rangle$ . This indication of turbulence<br>breakdown is consistent with the runaway decrease in breakdown is consistent with the runaway decrease in  $Re<sub>L</sub>$  for  $Re<sub>L</sub> \le 150$ . As a result of our analysis, we can rule out a transition in the dominant balance of the  $\langle b'w' \rangle$  budget: at increasing stratification, the buoyancy<br>destruction, term  $\langle b'^2 \rangle$  becomes dominating as the destruction term  $\langle b^2 \rangle$  becomes dominating as the buoyancy flux is limited by  $\langle \partial_z b \rangle$ , that is, the buoyancy flux and variance are not maximized simultaneously. This suggests that the buoyancy flux is not maximizing because of laminarization of the flow. Rather, laminarization occurs because the total buoyancy flux  $\phi_b < q_w$ at all times, which inevitably results in a continuous

<span id="page-8-2"></span>

FIG. 3. Time series of (a) the buoyancy fluctuations and (b) the turbulent buoyancy flux at  $z = h$  for all SC<sub>C</sub> at Re = 3500. Symbols are as in [Fig. 1.](#page-7-1)

decrease of  $\text{Re}_L$  (until the laminar limit has been reached). The qualitative changes in the flow when  $Re<sub>L</sub> \approx 150$  are also visible in [Fig. 2a](#page-8-1), in which an accelerated increase of  $\mathrm{Ri}_b$  is observed. The marked transition in the range  $\mathrm{Re}_L \approx$ 100–200 is consistent with the observations of earlier studies [\(Flores and Riley 2011](#page-20-9)).

#### <span id="page-8-0"></span>b. Neumann versus Dirichlet boundary conditions

The similarities of the above results with those by [Deusebio et al. \(2015\)](#page-20-11) encourage a more detailed comparison of the Couette flow when exposed to either Dirichlet or Neumann BCs. For this purpose, additional simulations have been performed, which are listed in [Table 2](#page-7-0). Excellent agreement (very closely overlapping lines) was obtained for the production and dissipation profiles between applying the different buoyancy BCs ([Fig. 4a\)](#page-9-0). Such agreement was found at  $Re = 1600$  and  $Re = 2500$  and for the other budget terms of the TKE (not shown). In terms of second-order quantities, the effect of the buoyancy BCs is limited to the near-wall region of  $\langle b^2 \rangle$  [\(Fig. 4b\)](#page-9-0). Further differences mainly manifest themselves in the (higher order) transport and redistribution terms of the  $\langle b'w' \rangle$  and  $\langle b'^2 \rangle$  budgets, but<br>even then the differences are most prominent below even then, the differences are most prominent below  $z/h \approx 0.15$ .

The differences occur because the Dirichlet BC enforces dissipation of any fluctuations of buoyancy at the wall by imposing a strong gradient locally. In the case of

<span id="page-9-0"></span>

FIG. 4. (a) The time-averaged production  $P_{\text{tke}}$  and dissipation  $\varepsilon_{\text{tke}}$  profiles of the TKE (as indicated in the figure) and (b) the timeaveraged dissipation  $\varepsilon_{bb}$  and turbulent transport  $T_{bb}$  terms of  $\langle b^2 \rangle$ . These terms represent the most dominant terms of each budget. The symbols indicate Neumann-BC cases R35S317 (black  $\Diamond$ ) and R35S237 (black +) and Dirichlet-BC cases R35R011 (red  $\Diamond$ ) and  $R35R037$  (red  $+$ ). The thin red lines show the instantaneous profiles to indicate the spread (only for cases R35R011 and R35SR037). The inset in (a) emphasizes the close agreement between BC types.

Neumann BCs, the gradient is fixed, and fluctuations of buoyancy may exist down to  $z = 0$ . The reasons that these differences do not show up in the TKE budget (i.e., via the buoyancy term in the  $\langle w^2 \rangle$  budget; see [Shah and](#page-21-18) [Bou-Zeid 2014\)](#page-21-18) are the no-penetration BC and that the additional  $\langle b^2 \rangle$  in the case of Neumann BCs is being dissipated in the near-wall region (see the peak of  $\varepsilon_{bb}$  at  $z/h \approx 0.04$  in [Fig. 4b\)](#page-9-0) instead of reaching the outer layer. The fact that the difference in buoyancy fluctuations does not seem to affect the other flow properties is important because it allows us to compare the first- and second-order (quasi-) steady-state statistics directly, regardless of the buoyancy BCs.

Since the steady states of the flux-driven simulations discussed above are essentially the same as corresponding cases using Dirichlet BCs, we expect that this similarity holds for all stably stratified Couette flow simulations with either Dirichlet or Neumann BCs. However, important differences may exist in terms of dynamic stability. In the Couette flow, this is mainly expressed at strong stratification, when the flow becomes intermittently turbulent. Based on the studies of [van de Wiel et al. \(2007\)](#page-21-5), [Taylor \(1971\)](#page-21-4), and [Phillips](#page-21-19) [\(1972\)](#page-21-19), we may formulate and test the following hypothesis: to the left of the maximum in [Fig. 5a](#page-10-1), the equilibriums are dynamically stable, while to the right, they are dynamically unstable in case the wall flux is imposed.

The point of departure is the relation between the turbulent buoyancy flux and the bulk Richardson number in a horizontally homogeneous flow. Given  $\text{Ri}_b$ (Dirichlet BC), a single steady state may be achieved in terms of the buoyancy flux corresponding to exactly one point on the curve in [Fig. 5a](#page-10-1) [\(Deusebio et al. 2015](#page-20-11); [Zhou](#page-21-7) [et al. 2017](#page-21-7)). Conversely, given  $q_w$  (Neumann BC), two, one, or zero turbulent equilibriums may exist in terms of  $\text{Ri}_b$ . If  $B_{\text{max}}/q_w < 1 \text{ (SC}_C < \text{SC}_C^{\text{crit}})$ , no turbulent solution exists and the flow laminarizes [\(van Hooijdonk et al.](#page-21-6) [2017b](#page-21-6)), where  $B_{\text{max}}$  is the maximum turbulent flux at  $z = h$  and  $B_{\text{max}} \simeq \phi_{b,\text{max}}$ , assuming negligible molecular transport at  $z = h$ . If  $B_{\text{max}}/q_w > 1$  (SC<sub>C</sub> > SC<sub>C</sub><sup>crit</sup>), two turbulent equilibriums exist (points 1 and 2 in Fig.  $5a$ ). Suppose the initial system state is given by the lower-left corner of the graph ( $\text{Ri}_b = 0$ ). Then the system evolves toward point 1, a dynamically stable equilibrium (indicated by the arrows). Following the RANS-based predictions of [van de Wiel et al. \(2007\),](#page-21-5) point 2 constitutes a dynamically unstable equilibrium. Thus, depending on the history and forcing of the flow, it will either evolve to point 1 or the flow will collapse toward its laminar equilibrium eventually.

To test this last assertion, the following experiment is conducted: Consider a state with a particular (mean)  $\mathrm{Ri}_b$ and a (mean)  $\langle b'w' \rangle$  corresponding to the right-hand side<br>(rbs) of the maximum in Fig. 5b (black circled dot) (rhs) of the maximum in [Fig. 5b](#page-10-1) (black-circled dot), which is used as initial condition for two simulations with new Neumann BCs:

- 1)  $B_{\text{max}}/q_w > 1 \wedge \langle b'w' \rangle_{t=0}/q_w < 1$  (SC<sub>C</sub> = 23.7; solid line in [Fig. 5b\)](#page-10-1),
- 2)  $B_{\text{max}}/q_w > 1 \wedge \langle b'w' \rangle_{t=0}/q_w > 1$  (SC<sub>C</sub> = 28.5; dotted line in [Fig. 5b\)](#page-10-1).

In both cases, dynamically stable, turbulent equilibriums exist, as found in [section 3a](#page-5-0). However, in the first case, we expect the system to collapse following the solid arrow. Conversely, in the second case, we expect that a

<span id="page-10-1"></span>

FIG. 5. Sketches of the steady-state relation between the turbulent buoyancy flux and the bulk Richardson number. Similar sketches were presented by [van Hooijdonk et al. \(2015\)](#page-21-3) and [Ansorge \(2017\)](#page-19-10). The shape of the curve to the right of the maxima is highly uncertain, since the flow is not horizontally homogeneous in this regime. (a) Sketch of the flow character at different stages. The black-circled dots represent conceptual equilibrium states for a specific (absolute value of) imposed wall flux (dashed line). (b) Sketch of the hypothesized evolution for two different imposed wall fluxes (represented by black horizontal lines) when the flow is initialized from a strongly stratified state (black-circled dot). The arrows indicate the hypothesized evolution for the two cases described in the main text: i.e., collapsing (solid) and recovering (dotted).

fully turbulent state is recovered following the dotted arrows.

The first simulation, with  $SC_C = 23.7$ , indeed shows a collapse (decreasing TKE, increasing  $Ri_b$ ; see [Fig. 6](#page-10-2)), despite the existence of a turbulent steady state for this value of  $SC<sub>C</sub>$  (cf. case R35S237 in [Fig. 2](#page-8-1)). For example, the magnitude of the fluctuations decreases three orders of magnitude between [Fig. 7a](#page-11-1) and [Fig. 7b.](#page-11-1) The second simulation shows different behavior. In this case, turbulence almost disappears, and  $Re<sub>L</sub>$  is temporarily less than 200. However, contrary to the first case, the bulk Richardson number now immediately decreases [\(Fig. 6](#page-10-2)),

<span id="page-10-2"></span>

FIG. 6. Time series of the TKE (left axis; symbol  $\Delta$ ) and  $\mathrm{Ri}_b$  (right axis; symbol  $\nabla$ ) for two cases with Re = 3500 initialized with a strongly stratified field, i.e., with  $\mathrm{Ri}_b$  belonging to the rhs of the maximum in [Fig. 5](#page-10-1). The colors indicate  $SC_C = 23.7$  (blue) and  $SC_C = 28.5$  (red).

followed by a recovery of turbulence at later times ([Fig. 7c\)](#page-11-1). This is also expressed in  $Re<sub>L</sub>$ , which is close to 500 at the end of the simulation. During the recovery, the buoyancy flux in the center temporarily reaches a value of  $\langle b'w' \rangle / q_w \approx 2$  (not shown). This high value is the result of the initial coexistence of recovering turbulance result of the initial coexistence of recovering turbulence (increasing mixing lengths) and a strong buoyancy gradient, such that each of the newly generated eddies carries extra buoyancy. An interesting observation is that a narrow band along the streamwise direction remains in which turbulence does not recover, at least within the simulated time ([Fig. 7c\)](#page-11-1). The most likely explanation is that  $\text{Ri}_b$  is still quite high for a DNS ( $\sim$ 0.04) at the end of the run, in combination with the periodic BCs that allow self-reinforcement of the nonturbulent band. These self-reinforcing bands were also observed in literature [\(Flores and Riley 2011](#page-20-9); [Deusebio et al. 2015](#page-20-11)).

The distinct behavior between these simulations pins down a clear dependence on the initial conditions when employing Neumann BCs in a Couette flow. In the Dirichlet case, similar behavior cannot occur, since for given Re and Pr, a unique (in terms of statistical properties) solution exists for each value of  $\mathrm{Ri}_b$  ([Deusebio](#page-20-11) [et al. 2015](#page-20-11)). Within the atmospheric context, these results are also consistent with the linear stability analysis of [van de Wiel et al. \(2017\)](#page-21-2). This study coupled the choice of BC to a physically relevant case; that is, Neumann and Dirichlet conditions correspond to fresh and melting snow, respectively.

## <span id="page-10-0"></span>c. Reynolds number dependence of the critical shear capacity

Several variables exemplify a transition from a fully turbulent steady state to a state of decaying turbulence or laminarization in the range  $SC_C \approx 22-24$  [\(Figs. 8a,b](#page-12-0)). Moreover, for a given  $SC<sub>C</sub>$ , the velocity fluctuations

<span id="page-11-1"></span>

FIG. 7. Instantaneous visualization of horizontal cross sections of the vertical velocity fluctuations at  $z = h$  from two cases with  $Re = 3500$  initialized with the same strongly stratified field. (a) The initial field at  $t = 0$  for both cases. At  $tU_0/h = 400$ , (b) the velocity field at when  $SC_C = 23.7$  and (c) the velocity field when  $SC_C = 28.5$ . In (a) and (c), the scale ranges between  $w/U_0 = \pm 0.05$ . In (b), the shades span a range of w that is two orders of magnitude lower than in the other figures.

and the bulk Richardson number are almost independent of Re when  $SC_C \gtrsim 24$  and Re  $> 1600$ . A closer look at the "critical range" suggests a small dependence of  $SC_C^{crit}$  on Re, which is further investigated below.

In most cases, classification as either becoming statistically steady or collapsing is straightforward since, for example, at  $SC_C = 31.7$ , all cases show statistical steadiness during several hundred  $h/U_0$ , while when  $SC_C \leq 22.0$ , a clear collapse occurs at each Re considered. When  $SC_C$  is closer to  $SC_C^{crit}$ , a more detailed classification is needed. For this purpose, we analyze two quantities in more detail. First, we investigate the planeaveraged total buoyancy flux in the center of the flow  $\langle \phi_b \rangle_{z=h}$ . Maximization of  $\langle \phi_b \rangle_{z=h}$  [\(Fig. 9a](#page-12-1)) followed by a decrease (i.e., the rhs of the maximum in [Fig. 5](#page-10-1) is reached) indicates that the flow is incapable of matching the BCs (see example cases in [Fig. 3](#page-8-2)).

<span id="page-11-2"></span>As a second quantity, we use the normalized buoyancy flux, such that it represents correlation between  $b'$ and w' (also at  $z = h$ ), defined as

$$
a_{bw} = \frac{|\langle b'w'\rangle|}{(\langle b'^2 \rangle \langle w'^2 \rangle)^{1/2}}.
$$
 (9)

This parameter takes an apparently universal value of approximately 0.4–0.45 when the flow is only neutrally or weakly stratified and  $Re$   $>$  1600. This value was also found, for example, in an LES of a plane channel flow [\(Armenio and Sarkar 2002](#page-19-3)), in a DNS of a stably stratified Ekman flow ([Ansorge and Mellado 2016\)](#page-19-1), and in a DNS of a stably stratified shear flow ([Jacobitz et al.](#page-20-24) [1997\)](#page-20-24). When  $SC_C < SC_C^{crit}$ , a strong decrease of  $a_{bw}$  occurs after some time, which signals a collapse of turbulence [\(Fig. 9b\)](#page-12-1). The subsequent irregular behavior is a consequence of small values of  $\langle b^2 \rangle$  and  $\langle w^2 \rangle$ . When  $SC_C \approx SC_C^{\text{crit}}$ , we may not obtain a definite answer from our simulations. In these cases (particularly at larger Re), the flow neither shows signs of a collapse nor of steadiness within the simulated time.

An overview of the classification of all cases ([Fig. 10](#page-13-1)) reveals that the critical shear capacity decreases with increasing Re up to  $Re = 3500$ . Beyond this threshold, such clear dependence is not observed. A few cases in a very narrow range around  $SC_C^{crit}$  remain nonstationary, that is, they are neither in steady state nor collapsing, which may obscure a possible weak dependence in the relatively high Re range.

## <span id="page-11-0"></span>d. Interdependency of the Obukhov–Reynolds number and the buoyancy flux

Once  $Re_L \le 100$ ,  $a_{bw}$  decreases sharply, indicating decorrelation of the vertical velocity and temperature fluctuations, which is a sign of collapsing turbulence ([Fig. 11a](#page-13-2), shown for Re  $\geq$  2500 only). Below Re<sub>L</sub>  $\approx$  40, the behavior is erratic, because  $\langle b^2 \rangle$  and  $\langle w^2 \rangle$  become small. The overall shape of the curve is independent of Re.

The temporal behavior of individual variables corroborates previous observations of a characteristic value of  $\text{Re}_L$  marking the transition to intermittent or laminar flow in the Couette, channel and Ekman flow ([Deusebio](#page-20-11) [et al. 2015](#page-20-11); [Flores and Riley 2011](#page-20-9); [Ansorge 2017\)](#page-19-10), as is indicated by an example case in [Fig. 11b](#page-13-2). Once  $Re<sub>L</sub>$ decreases below approximately 200,  $\langle w^2 \rangle$  declines gradually in time and more rapidly later, particularly when  $Re<sub>L</sub>$ is less than 100. Simultaneously,  $\langle \partial_z b \rangle_{z=h}$  increases more rapidly, and the evolution of  $\langle b^2 \rangle^{1/2}$  changes from increasing to decreasing.

While the onset of intermittency is marked by a narrow range of  $Re<sub>L</sub>$ , the turbulent buoyancy flux  $|\langle b'w' \rangle|$  maximizes in the range Re<sub>L</sub>  $\approx$  200–700, depending on Re (Fig. 12a). This maximum precedes pending on Re ([Fig. 12a](#page-14-0)). This maximum precedes, rather than follows, the transition, provided Re is large enough. However, at intermediate Re, the

<span id="page-12-0"></span>

FIG. 8. The final state of (a)  $\langle w^2 \rangle / u^2_r$  and (b)  $\text{Ri}_b$  for each case as invertion of SC<sub>e</sub>. The trail visualizes the evolution during the final a function of  $SC_C$ . The trail visualizes the evolution during the final  $100h/U_0$  to indicate (non)steadiness of the flow. The inset in (b) shows an enlargement of the overlapping symbols at  $SC_C = 31.7$ . (c) Each color represents a value of Reshown in (a) and (b). Each symbol corresponds to a value of SC<sub>C</sub>: 31.7 ( $\Diamond$ ), 27.1 ( $\nabla$ ), 25.2 (\*), 24.4 ( $\circ$ ), 23.7 (+), 23.1 ( $\times$ ), 22.5 ( $\times$ ), 22.0 ( $\Delta$ ), and 21.5 ( $\star$ ).

intermittency boundary may be crossed before the buoyancy flux maximizes.

We observe such behavior at Re = 1600 and  $SC_C = 23.7$ (case R16S237). This case is run for an extended period until  $t = 2500h/U_0$  ( $\approx 110h/u_\tau$ ). During this period, flow rearranged into persistent turbulent/nonturbulent bands (as in [Deusebio et al. 2015;](#page-20-11) not shown). A similar tendency was observed at  $Re = 1000$  (cases R10S244 and R10S237), although the simulation lengths were much shorter for these cases. As such, a statistically steady intermittent state can exist at low Re despite the use of Neumann BCs. This implies that the concepts discussed with respect to [Fig. 5](#page-10-1) are only valid at sufficiently high Re.

The curves on the (strongly stratified) left-hand side (lhs) of the maximum in [Fig. 12a](#page-14-0) lie much closer

<span id="page-12-1"></span>

FIG. 9. (a) The maximum instantaneous value of the total buoyancy flux  $\langle \phi_b \rangle_{z=h}$  that occurs during the entire simulation. (b) Temporal evolution of the  $b'$ –w' correlation  $[(9)]$  $[(9)]$  for a collapsing and a steady-state case for each Reynolds number considered. Colors are as in [Fig. 8.](#page-12-0) Each symbol corresponds to a value of  $SC_C$ :  $31.7 \ (\diamondsuit), 27.1 \ (\nabla), 25.2 \ (*), 24.4 \ (\odot), 23.7 \ (+), 23.1 \ (\times), 22.5 \ (\triangleright),$ 22.0 ( $\Delta$ ), and 21.5 ( $\star$ ).

together than on the (weakly stratified) rhs, where the shape of the curves is dependent on Re and  $SC<sub>C</sub>$ . This indicates that  $Re<sub>L</sub>$  appropriately characterizes the strongly stratified Couette flow. Conversely, the weakly stratified side shows more scatter, which may be explained by the notion that a turbulent stratified flow requires more than one parameter to characterize the flow under all stability conditions [\(Shih et al. 2005;](#page-21-15) [Brethouwer et al. 2007\)](#page-19-7). Alternatively, the larger scatter here may be due to the initial transient, since the flow is initialized on the weakly stable side of the maximum (see [section 3e](#page-13-0)).

A pivotal parameter to assess the dynamical stability of the system from its external parameters is the value of the Obukhov–Reynolds number that yields the maximum buoyancy flux. [Figure 12b](#page-14-0) shows that this value increases as a function of Re, which is supported by theoretical analysis of a bulk model. In the limit of

<span id="page-13-1"></span>

FIG. 10. Overview of all runs in the  $Re-SC_C$  plane. The runs are classified by the following symbols: Circles represent cases that are in a turbulent steady state. Crosses show a significant decrease in TKE and a similar increase of  $\mathrm{Ri}_b$ , which is associated with a collapse. The squares indicate cases that did not become steady within the simulated time but also did not show signs of a collapse of turbulence.

<span id="page-13-3"></span>large Re, this analysis yields (see [appendix C](#page-17-2) for a derivation)

$$
\text{Re}_{L} \sim \frac{27\alpha}{4\kappa} \frac{\text{Re}_{\tau}}{\ln(\text{Re}_{\tau})}.
$$
 (10)

Since  $\text{Re}_{\tau}$  increases with  $\text{Re}$ , [\(10\)](#page-13-3) shows that the value  $Re<sub>L</sub>$  at the maximum buoyancy flux is an increasing function of Re within the limits of these derivations. Additionally, the obtained relation suggests that at low Re, near-wall processes become limiting  $[i.e., Re<sub>L</sub>]$ becomes less than  $O(10^2)$ ] before  $\phi_h$  reaches its maximum value based on the global constraint that scales as  $U_0^3/h$ . At larger Re, the buoyancy flux maximizes when  $Re<sub>L</sub> > O(10<sup>2</sup>)$ , which marks the onset of positive feedback toward  $Re_L \sim O(10^2)$  and thus toward laminarization.

To obtain a quantitative estimate of  $Re<sub>L</sub>$  when  $\phi_b = \phi_{b, \text{max}}$ , we need to know the functional dependence of  $\text{Re}_{\tau}$  on  $\text{Re}$  and  $\text{Ri}_b$ . For specific Re and  $\text{Ri}_b$ , the value of  $\text{Re}_{\tau}$  may be estimated using Monin–Obukhov similarity theory (MOST) extended with an appropriate wall model (e.g., [van Driest 1956](#page-21-20)). Alternatively, the values as listed in [Table 1](#page-6-0) may be used. This indicates that, indeed, the value of  $Re<sub>L</sub>$  at the transitional SC<sub>C</sub> increases with Re. It also suggests that at the transition point  $Re<sub>L</sub> > O(10<sup>2</sup>)$  when  $Re > O(10<sup>3</sup>)$ , meaning that the presently used Re are only just sufficient to observe the flux maximum resulting from a global constraint. Moreover,  $(10)$  suggests that the value of  $Re<sub>L</sub>$  at the flux maximum increases slowly with increasing Re and that a very large value of Re is required to observe  $Re_L \gg$ <br> $O(100)$  at  $SC = SC<sup>crit</sup>$ </sup>  $O(100)$  at SC<sub>C</sub> = SC<sub>C</sub><sup>crit</sup>.

<span id="page-13-2"></span>

FIG. 11. (a) The correlation between fluctuations of buoyancy and the vertical velocity as function of  $Re<sub>L</sub>$ . The trail of lighter symbols visualizes the temporal behavior with a thick symbol marking the end point of each simulation. Colors are as in [Fig. 8c](#page-12-0). Each symbol corresponds to a value of SC<sub>C</sub>: 31.7 ( $\diamond$ ), 27.1 ( $\nabla$ ), 25.2 (\*), 24.4 (O), 23.7 (+), 23.1 ( $\times$ ), 22.5 ( $>\rangle$ ), 22.0 ( $\Delta$ ), and 21.5  $(\star)$ . For clarity, the data for Re = 1000 and Re = 1600 are not shown. See [appendix B](#page-17-1) ([Fig. B1a](#page-19-12)) for a comparison with data from an Ekman flow. (b) Time series of the buoyancy fluctuations (black; left axis), the vertical velocity fluctuations (red; right axis), and the buoyancy gradient at  $z = h$  (blue; right axis) for Re = 3500 with  $SC_C = 21.5$ . The vertical lines highlight the time when  $Re_L = 200$ and  $Re<sub>L</sub> = 100$ .

#### <span id="page-13-0"></span>e. Richardson number versus buoyancy flux

In this section, we investigate if the occurrence of a maximum turbulent buoyancy flux can be characterized by a Richardson number. The maximum buoyancy fluxes at  $Re = 1000$  (dark red) and  $Re = 1600$  (black) are significantly lower than at larger Re (Fig.  $13a$ ). For increasing Re,  $\langle b'w' \rangle_{\text{max}}$  becomes progressively less sen-<br>sitive to Be, which is suggesting convergence sitive to Re, which is suggesting convergence.

While the value of the maximum flux may become independent of Re, the bulk Richardson number associated with the maximum does not show a similar convergence (at least at the present Re). This appears to contradict MOST-based prediction using a bulk model of a Couette flow with rough walls [\(van de Wiel](#page-21-12) [et al. 2012b\)](#page-21-12), where the maximum was associated with  $\text{Ri}_b = 1/(3\alpha)$ , with  $\alpha$  a fit parameter for the Businger– Dyer flux–profile relations [\(Businger et al. 1971\)](#page-19-11). Possibly

<span id="page-14-0"></span>

FIG. 12. (a) The buoyancy flux as function of  $Re<sub>L</sub>$ . The trail of lighter symbols visualizes the temporal behavior, with a thick symbol marking the end point of each simulation. Colors are as in [Fig. 8c.](#page-12-0) Each symbol corresponds to a value of  $SC_C$ : 31.7 ( $\diamond$ ), 27.1  $(\nabla)$ , 25.2 (\*), 24.4 (O), 23.7 (+), 23.1 (×), 22.5 (>), 22.0 ( $\Delta$ ), and 21.5 ( $\star$ ). (b) Evolution of  $\langle b'w' \rangle$  for Re = 1600 (black), 2500 (blue),<br>3500 (red), and 4500 (green) and SC = 22.5. Vertical line indicates 3500 (red), and 4500 (green) and  $SC_C = 22.5$ . Vertical line indicates the time when  $Re<sub>L</sub> = 200$  for each Reynolds number with the corresponding color.

the difference exists because the bulk model neglects the viscous damping in the buffer layer. Additionally, the model considers only one flux–profile relation. Others may show more complex dependency on  $z_0$  [\(Holdsworth](#page-20-21) [et al. 2016\)](#page-20-21), particularly when  $z_0$  is low (as is the case for smooth DNS wall).

Contrary to  $\mathrm{Ri}_b$ , the local gradient Richardson number Ri at  $z = h$  attains a unique value of Ri  $\approx 0.1$  at the maximum, with only a slight increasing tendency for larger Re [\(Fig. 13b\)](#page-14-1). Particularly on the weakly stratified side of the maximum, the steady-state values (large symbols) in the  $[Ri - \langle b'w' \rangle]$  plane form a single curve.<br>This is consistent with the assumption of Phillips (1972) This is consistent with the assumption of [Phillips \(1972\)](#page-21-19) that the buoyancy flux can be expressed in terms of local gradients. Conversely, on the rhs, the data do not collapse, indicating that local gradients are no longer

<span id="page-14-1"></span>

FIG. 13. The mean turbulent buoyancy flux between  $z = 0$ and  $z = h$  as function of the (a) bulk Richardson number and (b) gradient Richardson number at  $z = h$ . The trail of lighter symbols visualizes the temporal behavior, with a thick symbol marking the end point of each simulation. Colors are as in [Fig. 8c](#page-12-0). Each symbol corresponds to a value of SC<sub>C</sub>: 31.7 ( $\diamond$ ), 27.1 ( $\nabla$ ), 25.2 (\*), 24.4 (O), 23.7 (+), 23.1 ( $\times$ ), 22.5 ( $>\rangle$ ), 22.0 ( $\Delta$ ), and 21.5  $(\star)$ . For clarity, the data for Re = 1000 and Re = 1600 are not shown in (b).

representative of the local flux. In the limited context of the current low-Re DNS, no specific critical bulk Richardson number could be discerned marking the transition from WSBL to VSBL.

Finally, we observe that for the lowest  $SC_C$ , the maximum buoyancy flux is not reached (e.g., when  $Re = 6200$ ,  $SC_C = 21.5$ ; light-blue star in [Fig. 13a\)](#page-14-1). The initial turbulence is damped so strongly that the simulation enters straight into the slow evolution on the strongly stratified side of the maximum buoyancy flux. From a MOST perspective, each value of Ri is associated with a single value of the buoyancy flux (for a specific value of Re) since turbulence is always in instantaneous equilibrium with the mean flow. A consequence is that, within the MOST framework, the flow should trace the same curve in [Fig. 13a](#page-14-1), irrespective of  $SC<sub>C</sub>$  (but not necessarily of Re). Interestingly, the turbulent buoyancy flux at  $z = h$  initially follows the line  $\langle b'w'\rangle h/U_0^3 \approx 3 \times 10^{-4}$ Ri for each case ([Fig. 13b\)](#page-14-1). How-<br>over this line is not close to the equilibrium curve (the ever, this line is not close to the equilibrium curve (the virtual line interpolating the thick symbols in [Fig. 13b](#page-14-1) at  $\text{Ri} \leq 0.1$ ). When  $\text{SC}_C > \text{SC}_C^{\text{crit}}$ , the equilibrium curve is reached after some time following a line of constant Ri, while the buoyancy flux is still increasing. The fact that we observe all cases following a different curve from the equilibrium curve indicates limited applicability of MOST-based parameterizations for a fast-evolving environment [\(Nadeau et al. 2011](#page-20-25); [van Hooijdonk et al.](#page-21-21) [2017a](#page-21-21)). When  $SC_C < SC_C^{\text{crit}}$ , the temporal evolution traces a complex line in the  $\text{Ri} - \langle b'w' \rangle$  plane, which is associated<br>with the onset of intermittent flow with the onset of intermittent flow.

## <span id="page-15-0"></span>4. Discussion

Above, we relate the occurrence of a maximum buoyancy flux to a global constraint (expressed by  $SC_C$ ) and to wall dynamics (expressed by  $Re<sub>L</sub>$ ). Below, the occurrence of this maximum in the present results is discussed in relation to previous studies. Regarding the kind of BC, the equilibrium may depend on the initial turbulent buoyancy flux for Neumann-type BCs, which is consistent with theoretical considerations on the maximum buoyancy flux. Such a dependency is not found for Dirichlet-type BCs. [Section 4b](#page-16-1) elaborates on how this result may be extended to other flow configurations.

### a. Parameters for the collapse of turbulence

The existence of a maximum buoyancy flux finds support from theoretical work [\(Taylor 1971](#page-21-4); [Phillips](#page-21-19) [1972;](#page-21-19) [van de Wiel et al. 2007;](#page-21-5) [Caulfield and Kerswell](#page-19-13) [2001\)](#page-19-13), from field observations in the atmosphere and in the ocean ([Posmentier 1977](#page-21-22); [Malhi 1995;](#page-20-8) [Monahan et al.](#page-20-7) [2015;](#page-20-7) [van Hooijdonk et al. 2015](#page-21-3)), and from laboratory experiments ([Linden 1979;](#page-20-26) [Holford and Linden 1999](#page-20-27)). A main point of discussion is how the occurrence of this maximum is properly characterized and whether the buoyancy flux decreases when stratification becomes even stronger.

The present results extend previously obtained insight into the merits of three distinct parameters and into their relation to each other.

• The Obukhov–Reynolds number  $Re<sub>L</sub>$  is related to the turbulent fraction at strong stability. Consistent with the present results, earlier studies observed relaminarization of the flow in the plane channel flow [\(Flores](#page-20-9) [and Riley 2011](#page-20-9)), the Couette flow ([Deusebio et al.](#page-20-11) [2015\)](#page-20-11), and the Ekman flow [\(Ansorge 2017](#page-19-10)) once  $Re_L \le 100 - 200$ . In the Ekman flow, the turbulent fraction depended on the initial conditions when  $Re<sub>L</sub>$ was in the range of 200–800.

- The shear capacity  $SC<sub>C</sub>$  is an external bulk parameter for the Couette flow with Neumann BCs. It indicates whether the final state of this flow is turbulent or laminar, that is, whether or not the intermittency boundary at  $\text{Re}_L \approx O(100)$  will be reached (for large Re). In other configurations, SC separates the weakly stratified regime in which the buoyancy flux increases with increasing stratification from the strongly stratified regime in which the opposite is observed. In the flux-driven plane channel flow ([Nieuwstadt 2005;](#page-20-28) [Flores and Riley 2011](#page-20-9); [Donda et al. 2015\)](#page-20-22) or Ekman flow [\(Gohari and Sarkar 2017](#page-20-14)), the flow may only collapse temporarily, and  $SC<sub>C</sub>$  could be used to anticipate this temporary collapse [\(Donda et al. 2015](#page-20-22)).
- The gradient Richardson number Ri characterizes mixing in the weakly stratified flow ([Komori et al.](#page-20-29) [1983\)](#page-20-29) in a statistically steady state. At each vertical level, it also appears to appropriately characterize the maximum buoyancy flux, which at  $z = h$  occurs around  $Ri = 0.1$ . Although in a broad sense, turbulence is suppressed more at larger Ri, the mixing is no longer appropriately characterized by Ri in a strongly stratified flow. As such, the collapse of turbulence cannot be associated with a single value of Ri in a wallbounded flow, consistent with the argument of [Shih](#page-21-15) [et al. \(2005\)](#page-21-15).

Thus,  $SC<sub>C</sub>$  describes the mechanism leading to the eventual collapse, not the mechanism of the collapse itself. The value of  $Re<sub>L</sub>$  at the flux maximum depends on the bulk Reynolds number, which also means that for larger Re, it takes longer for the flow to laminarize after the maximum was reached (e.g., Fig.  $13$ ). Finally, the gradient Richardson number appears as a heightdependent and Re-independent parameter to characterize the occurrence of the maximum buoyancy flux. We note that all three of these parameters ( $Re<sub>L</sub>$ ,  $SC<sub>C</sub>$ , Ri) may be used to discriminate between stability regimes. While this appears unproblematic well within either weak or strong stability, our analysis demonstrates that close to the transition, the attribution of a case to weak or strong stability may critically depend on both the choice of the parameter and the turbulence scale separation. This leaves the question of how these fundamental results may be extended to the collapse of turbulence in reality. With respect to the actual turbulence collapse, earlier results [\(van Hooijdonk et al. 2015;](#page-21-3) [Monahan et al. 2015](#page-20-7)) show that the VSBL and WSBL are better characterized by the shear capacity than by, for example, a Richardson number. As such, the shear capacity provides insight into the mechanism leading to strongly stratified conditions. With respect to  $Re<sub>L</sub>$ , [Flores and Riley \(2011\)](#page-20-9) hypothesized that the  $Re<sub>L</sub>$  criterion could also be extended to flows over a rough surface based on observational data from the CASES-99 experiment [\(Poulos et al. 2002](#page-21-23)). This promising hypothesis requires further investigation since it is based on estimates of the boundary layer height (based on the near-surface wind speed) and the surface roughness. Both of these estimates become questionable under strongly stratified conditions. Nonetheless, the importance of near-wall processes in the critical regime of  $Re<sub>L</sub>$  (as explored in [section 3d\)](#page-11-0) actually supports that in a real SBL roughness plays a major role in the collapse or maintenance of turbulence. Hence, the roughness elements may define the scale separation instead of the Kolmogorov length scale [\(Ghannam et al.](#page-20-30) [2018\)](#page-20-30). This speculation is corroborated by the orderof-magnitude agreement between  $Re<sub>L</sub>$  found in numerical studies at moderate Reynold numbers and the real-world SBL ([Flores and Riley 2011](#page-20-9)). It remains, however, unclear how the production of turbulence (i.e., in the buffer layer in traditional wall unit scaling) scales when normalized with a roughness scale.

#### <span id="page-16-1"></span>b. Similarity between boundary conditions

Wall-bounded turbulent flows under neutral stratification have many characteristics that are independent of the particular flow geometry ([Kim et al. 1987;](#page-20-10) [Spalart](#page-21-24) [1988\)](#page-21-24). In fact, characteristics persist in stable conditions when properly scaled in wall units. This is one reason underlying the success of MOST in both realistic ([Monin](#page-20-5) [1970;](#page-20-5) [Holtslag et al. 2013](#page-20-20); [Mahrt 2014](#page-20-31)) and idealized flows (Garcí[a-Villalba and del](#page-20-15) Álamo 2011; [Donda et al.](#page-20-22) [2015;](#page-20-22) [Deusebio et al. 2015;](#page-20-11) [van Hooijdonk et al. 2017b;](#page-21-6) [Zhou et al. 2017](#page-21-7)). Considering this generality, the BC type is likely of limited importance in a steady state, at least on the weakly stratified side of the buoyancy flux maximum and  $Re_L \gg O(100)$ .<br>While in equilibrium different

While in equilibrium, differences in the higher-order statistical quantities may not affect the mean-flow properties; in strongly perturbed situations, such differences could play a role, as was suggested by [Jensen](#page-20-32) [et al. \(2016\)](#page-20-32), for the sunset period. Moreover, important differences in dynamical behavior of the mean flow can arise in a Couette flow, and it is natural to explore these differences in configurations other than the Couette flow as well. Previous studies (e.g., [Garg et al. 2000;](#page-20-17) [Flores](#page-20-9) [and Riley 2011](#page-20-9); Garcí[a-Villalba and del](#page-20-15) Álamo 2011; [Donda et al. 2015\)](#page-20-22) support a similar rationale for the plane channel flow: In the case of Dirichlet BCs, an intermittent statistically steady state exists at strong stratification [\(Deusebio et al. 2015](#page-20-11)). In the case of Neumann BCs, such a state cannot be steady, since flow acceleration also reduces the bulk gradient.

[Gohari and Sarkar \(2017\)](#page-20-14) performed a direct comparison using different buoyancy BCs for an Ekman flow. They made the comparison at times when the bulk Richardson number (based on the neutral Ekman-layer depth) of the Neumann case was instantaneously equal to the long-time quasi-steady state of a Dirichlet case. The mean horizontal velocity components showed poor agreement between the two types of boundary conditions. This poor agreement may be explained partially by the significant difference in  $u_{\tau}$ . The TKE profiles showed reasonable agreement once normalized with  $u_{\tau}$ and only when TKE was strong, which in fact further supports scaling in wall units. When TKE was weak, poor agreement was found, which may be explained by the intermittent, and thus statistically inhomogeneous, character of the flow. It would be interesting to revisit this analysis to compare the BCs systematically when the flow is in a similar quasi-steady state in terms of  $\text{Re}_\tau$ .

While the considerations above raise concerns of caution for transient flow configuration, studies of the equilibrium flow may opt for the buoyancy BC that best suits their purposes. Dynamically, however, crucial differences become apparent even in conceptual configurations. While both Neumann and Dirichlet BCs yield important mechanical insight, neither is necessarily more realistic or more suitable than the other. Therefore, if a realistic nonstationary setup is aimed for, the coupling to a surface energy budget is inevitable.

#### <span id="page-16-0"></span>5. Conclusions

Direct numerical simulations of the stably stratified Couette flow have been performed. We quantified the Reynolds number dependence of the buoyancy flux maximum dependency on the Obukhov–Reynolds number. Findings by [van Hooijdonk et al. \(2017b\)](#page-21-6) are confirmed on a range of Re and on a larger domain. The results show that in a steady state, most first- and secondorder statistical quantities are indistinguishable between a Couette flow with Neumann BCs or with Dirichlet BCs. Dynamically, however, differences become apparent that are consistent with the prediction on the dynamic stability of the flow ([Phillips 1972](#page-21-19); [Posmentier 1977;](#page-21-22) [van de Wiel et al. 2007\)](#page-21-5). In the range  $\text{Re} \approx 1000-3500$ , stronger dependence on Re is observed, but at larger Re, the value of SC $_C^{\rm crit}$  appears to converge to approximately 23. We showed theoretically that convergence of  $\mathrm{SC}_\mathcal{C}^\mathrm{crit}$  is inconsistent with convergence in terms  $Re<sub>L</sub>$ . Based on analytical considerations, we showed that the occurrence of a maximum buoyancy flux is not controlled by

wall dynamics but rather that it follows from a global constraint. This is consistent with earlier theoretical predictions for the Couette flow by [Caulfield and Kerswell](#page-19-13) [\(2001\)](#page-19-13) and [van de Wiel et al. \(2007\).](#page-21-5) However, consistent with [Flores and Riley \(2011](#page-20-9); and later studies), we find that the collapse of turbulence occurs when  $Re_L \approx 100-200$ . This means that the global constraint inevitably leads to a collapse of turbulence, which actually occurs because of suppression of near-wall structures.

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## APPENDIX A

#### Resolution Overview

<span id="page-17-0"></span>[Table A1](#page-18-0) provides an overview of the resolution for each simulation. The resolution is based on steady-state measurements of  $u_{\tau}$ . If the simulation did not reach a steady state, the resolution was estimated using the steady-state values of a run with the same Re and a larger value of  $SC<sub>C</sub>$  (i.e., less stratified).

### APPENDIX B

#### Comparison to the Ekman Flow

<span id="page-17-1"></span>In this paper, we have chosen the Couette flow as the main object of interest for its conceptual simplicity. This conceptual approach necessitates the neglect of important physical mechanisms when considering real atmospheric conditions. A step toward more realistic but not yet atmospheric—conditions may be made by comparing our results to the statistics of the Ekman flow, thus incorporating the effects of rotation, a pressure gradient, and breaking the vertical symmetry. However, a one-to-one comparison is complicated by several factors, such as nonsteadiness of the Ekman flow. Therefore, we compare the flow statistics in the surface layer only. For this purpose, the budget terms of the TKE are defined as

- Shear production  $P_{\text{tke}} = \langle u'w' \rangle \partial_z U$ ,<br>Niscous transport  $V_{\text{t}} = u \partial_z \partial_x / u'^2 \partial_y$
- Viscous transport  $V_{\text{tke}} = \nu \partial_z \partial_z \langle u_i^2 \rangle$ ,
- Pressure transport  $\Pi_{\text{tke}}^T = -2\partial_z \langle p'w' \rangle$ ,<br>• Turbulent transport  $T_{\text{t}} = \partial_z \langle p'w' \rangle$
- Turbulent transport  $T_{\text{tke}} = \partial_z \langle u_i^2 w' \rangle$ ,
	- Dissipation  $\varepsilon_{\text{tke}} = -2\nu \langle (\partial_z u'_i)^2 \rangle$ .

Under neutral stratification, the budget terms of the TKE ([Fig. B1a](#page-19-12)) are independent of Re (for Re  $>$ 1600), and they match closely with previous results for the Ekman flow ([Ansorge and Mellado 2016\)](#page-19-1). This validates our numerical method and provides a further example of the similarity between wallbounded turbulent flows. For fixed-height statistics, the level  $zu_\tau/v = 30$  has been chosen, which is at the lower end of the logarithmic region. Therefore, surface-layer scaling should be valid, while external effects that are not present in the Couette flow are minimal. The comparison in [Fig. B1b](#page-19-12) is an illustrative example of more general applicability of the findings that have been discussed in depth for the Couette flow.

#### APPENDIX C

#### Theoretical Considerations

<span id="page-17-2"></span>The study of [Flores and Riley \(2011\)](#page-20-9) and the results of [van Hooijdonk et al. \(2015,](#page-21-3) [2017b\)](#page-21-6) suggest different criteria indicating the collapse of turbulence. [Flores](#page-20-9) [and Riley \(2011\)](#page-20-9) base their criterion on whether turbulence can be sustained by near-wall processes, while in [van Hooijdonk et al. \(2015\)](#page-21-3), a global constraint on the buoyancy flux is defined. The results of the previous sections provide support for both criteria and that they are applicable to different stages of the collapse.

Here, we aim for a qualitative relation for  $Re<sub>L</sub>$  as function of Re at the point where  $SC_C = SC_C^{crit}$  to investigate theoretically if  $\text{Re}_L$  and  $\text{SC}_C^{\text{crit}}$  are compatible criteria. Moreover, qualitative analytical insight into the Re dependence of the  $Re<sub>L</sub>-SC<sub>C</sub>$ relation supports the interpretation of the DNS results. First, we estimate the maximum total buoyancy flux  $\phi_{b,\text{max}}$  at  $z = h$  following a similar route as in earlier studies ([van de Wiel et al. 2012b](#page-21-12); [van](#page-21-3) [Hooijdonk et al. 2015;](#page-21-3) [van de Wiel et al. 2017](#page-21-2)), followed by an estimate of  $Re<sub>L</sub>$  under the assumption that  $\phi_b = \phi_{b,\text{max}} = q_w$ .

<span id="page-17-3"></span>The mean buoyancy evolution at a height  $z$  may be described by

$$
\partial_t b = -\partial_z \langle b' w' \rangle + \kappa_b \partial_z^2 b. \tag{C1}
$$

Next, [\(C1\)](#page-17-3) is integrated between  $z = 0$  and  $z = h$  and between  $z = h$  and  $z = 2h$ , resulting in

TABLE A1. Overview of the resolution in wall units for all simulations. Asterisks are as in [Table 1](#page-6-0).

<span id="page-18-0"></span>

Run	$\delta_x u_\tau$ $\nu$	$\delta_{y}u_{\tau}$ $\boldsymbol{\nu}$	$\delta_z u_\tau$ $\nu$	Run	$\delta_x u_\tau$ $\nu$	$\delta_{y}u_{\tau}$ $\nu$	$\delta_z u_\tau$ $\nu$	Run	$\delta_x u_\tau$ $\boldsymbol{\nu}$	$\delta_{y}u_{\tau}$ $\boldsymbol{\nu}$	$\delta_z u_\tau$ $\nu$
R10S271	2.7	2.7	0.8	R25S231*	3.7	3.3	1.1	R45S220**	3.9	3.7	$1.0\,$
R10S252	2.5	2.5	0.7	R25S225*	3.7	3.3	1.1				
R10S244*	2.5	2.5	0.7	R25S220*	3.7	3.3	1.1	R <sub>62</sub>	5.4	5.4	1.3
R10S237*	2.5	2.5	0.7					R62S317	5.0	5.0	1.2
				R35	4.8	4.4	1.4	R62S237	4.3	4.3	1.1
R <sub>16</sub>	3.5	3.5	1.0	R35S317	4.6	4.2	1.3	R62S231*	4.3	4.3	1.1
R <sub>16</sub> S <sub>317</sub>	3.4	3.4	1.0	R35S271	4.4	4.0	1.3	R62S225**	4.3	4.3	1.1
R16S252	3.1	3.1	0.9	R35S237	4.0	3.6	1.2	R62S215*	4.3	4.3	1.1
R <sub>16</sub> S <sub>244</sub>	3.0	3.0	0.9	R35S231*	4.0	3.6	1.2				
R <sub>16</sub> S <sub>237</sub> *	3.0	3.0	0.9	R35S225*	4.0	3.6	1.2	R <sub>16</sub> R <sub>009</sub>	3.4	3.4	1.0
R16S231*	3.0	3.0	0.9	R35S220*	4.0	3.6	1.2	R <sub>16</sub> R <sub>020</sub>	3.1	3.1	0.9
R <sub>16</sub> S <sub>225</sub> *	3.0	3.0	0.9	R35S215*	4.0	3.6	1.2	R <sub>25</sub> R <sub>010</sub>	4.3	3.8	1.3
R <sub>16</sub> S <sub>220</sub> *	3.0	3.0	0.9	R35S215*	4.0	3.6	1.2	R <sub>25</sub> R <sub>032</sub>	3.7	3.3	1.1
								R35R011	4.6	4.2	1.3
R <sub>25</sub>	4.5	4.0	1.3	R45	4.8	4.5	1.2	R35R037	4.0	3.6	1.2
R25S317	4.3	3.8	1.3	R45S317	4.5	4.2	1.1	R35VS285	4.0	3.6	1.2
R25S271	4.2	3.7	1.2	R45S237	3.9	3.7	$1.0\,$	R35VS237	4.0	3.6	1.2
				R45S231*	3.9	3.7	1.0				

<span id="page-18-1"></span>
$$
\partial_t \mathcal{B}_\downarrow = -\frac{1}{h} \int_0^h \partial_z \langle b' w' \rangle \, dz + \frac{1}{h} \int_0^h \kappa_b \partial_z^2 b \, dz, \quad (C2)
$$

$$
\partial_t \mathcal{B}_\uparrow = -\frac{1}{h} \int_h^{2h} \partial_z \langle b' w' \rangle \, dz + \frac{1}{h} \int_h^{2h} \kappa_b \partial_z^2 b \, dz, \quad (C3)
$$

in which  $\mathcal{B}_\downarrow = \int_0^h b \, dz/h$  and  $\mathcal{B}_\uparrow = \int_h^{2h} b \, dz/h$ . Continuing with the integrated buoyancy has the advantage that we do not need to treat the wall processes explicitly using a wall model; that is, we do not assume a specific shape of the velocity and buoyancy profiles.

<span id="page-18-4"></span>Combining [\(C2\)](#page-18-1) with the BCs  $(\langle b'w' \rangle = 0$  and  $\kappa_b \partial_z b =$  $-q_w$  at the walls) leads to,

$$
\partial_t \Delta \mathcal{B} \equiv \partial_t (\mathcal{B}_\uparrow - \mathcal{B}_\downarrow)/2 = q_w + h^{-1} \langle b'w' \rangle_{z=h}
$$

$$
-h^{-1} \kappa_b \partial_z b_{z=h}.
$$
 (C4)

<span id="page-18-2"></span>The fluxes are then modeled in bulk form,

$$
\langle b'w'\rangle_{z=h} = -\frac{\text{Re}_{z}^{2}}{\text{Re}^{2}}U_{0}\Delta\mathcal{B}f(\text{Ri}_{\mathcal{B}}),\tag{C5}
$$

$$
\kappa_b \partial_z b_{z=h} = \kappa_b \Delta \mathcal{B}/h,\tag{C6}
$$

<span id="page-18-3"></span>with  $f(Ri_{\mathcal{B}}) = (1 - \alpha Ri_{\mathcal{B}})^2$  the Businger–Dyer flux–<br>profile relations (Businger at al. 1971) and the Bishardson profile relations ([Businger et al. 1971](#page-19-11)) and the Richardson number based on the integrated buoyancy difference  $\text{Ri}_{\mathcal{B}} = h\Delta \mathcal{B}/U_0^2$ . The final result is only quantitatively sensitive to the specific choice of this function, provided it is a decreasing function of  $\text{Ri}_{\mathcal{B}}$ , which decreases faster than  $\mathrm{Ri}_\mathscr{B}^{-1}$  ([Derbyshire 1999\)](#page-19-9);  $\alpha \approx 5$  is a model parameter (Högströ[m 1996](#page-20-33)).

Equations  $(C5)$  and  $(C6)$  are then inserted into  $(C4)$ . Furthermore,  $(C4)$  is multiplied by  $h/U_0^3$ , and the steady state is assumed to arrive at the final dimensionless model equation

<span id="page-18-5"></span>
$$
\partial_{\tau} \Delta \text{Ri}_{\mathcal{B}} = 0 = -\frac{\text{Re}_{\tau}^{2}}{\text{Re}^{2}} \text{Ri}_{\mathcal{B}} f(\text{Ri}_{\mathcal{B}}) - \frac{\text{Ri}_{\mathcal{B}}}{\text{RePr}} + \frac{1}{\text{SC}_{C}^{3}}, \quad (C7)
$$

with  $\tau = tU_0/h$ .

Next, we assume that  $SC_C = SC_C^{\text{crit}}$ , that is,  $SC_C$  is such that the sum of the first two rhs terms in  $(C7)$ maximize. This maximum may be found by derivation with respect to  $\text{Ri}_{\mathcal{B}}$ . Since the mathematical structure of  $(C7)$  is very similar to the model equation of [van de Wiel et al. \[2017,](#page-21-2) their (2)], we do not repeat all steps here. A small difference with their derivation is that we do not assume that  $\text{Ri}_{\mathscr{B},\text{max}} = 1/(3\alpha)$ independently of Re, where the subscript ''max'' refers to a quantity that is measured when  $\phi_b = \phi_{b,\text{max}}$ . The result is

$$
\text{Ri}_{\mathcal{B},\text{max}} = \frac{2}{3\alpha} - \frac{1}{3\alpha} \mathcal{W},\tag{C8}
$$

with  $\mathcal{W} = \sqrt{1 - 3\text{Re}\text{Pr}^{-1}\text{Re}_\tau^{-2}}$ . Next, we estimate the relation between Re and  $\text{Re}_{\tau}$  using a logarithmic profile; that is,  $\text{Re} \sim \text{Re}_{\tau} \ln(\text{Re}_{\tau})$  ([Townsend 1976](#page-21-25)). This then leads to

$$
Re/Re_{\tau}^{2} \sim Re_{\tau} ln(Re_{\tau})/Re_{\tau}^{2},
$$
 (C9)

<span id="page-18-6"></span>which tends to 0 for  $\text{Re} \rightarrow \infty$ . Consequently, we recover the solution  $\text{Ri}_{\mathcal{B},\text{max}} \rightarrow 1/(3\alpha)$  of [van de Wiel et al.](#page-21-5) [\(2007\)](#page-21-5) when  $\text{Re} \rightarrow \infty$ . The corresponding maximum buoyancy flux is

<span id="page-19-12"></span>

FIG. B1. (a) Profiles of the TKE budget terms. Only results for  $Re = 1600$  (red) and  $Re = 6200$  (blue) are shown for clarity (for other Re, the results are virtually the same). The various terms are indicated in the figure. The solid black line represents results for the Couette flow at  $RE = 21 333$  obtained by [Pirozzoli et al. \(2014,](#page-21-26) production term only). The dotted black lines indicate results for the Ekman flow obtained by ([Ansorge and Mellado 2016,](#page-19-1) production and dissipation term). (b) Values at the end of each simulation, where the symbols indicate SC<sub>C</sub>: 31.7 ( $\diamond$ ), 27.1 ( $\nabla$ ), 25.2 (\*), 24.4 (O), 23.7 (+), 23.1 ( $\times$ ), 22.5 ( $\times$ ), 22.0 ( $\Delta$ ), and 21.5 ( $\star$ ). Black dots indicate the results for the Ekman flow, with  $SC<sub>C</sub>$  based on the geostrophic wind speed and an estimate of the boundary layer depth. Note that these data may be arbitrarily shifted within an order of magnitude by using different definitions of the boundary layer depth.

<span id="page-19-14"></span>
$$
\hat{\phi}_{b,\text{max}} = \frac{2 - \mathcal{W}}{27\alpha} \left[ \frac{9}{\text{PrRe}} + \frac{\text{Re}_\tau^2}{\text{Re}^2} (1 + \mathcal{W})^2 \right]. \quad (C10)
$$

Again, when  $\text{Re} \rightarrow \infty$ , the result of [van de Wiel et al.](#page-21-2) [\(2017](#page-21-2), and earlier papers) is retrieved:

$$
\lim_{\text{Re}\to\infty} \hat{\phi}_{b,\text{max}} = \frac{4\text{Re}_\tau^2}{27\alpha\text{Re}^2}.
$$
 (C11)

Finally, we may use [\(C10\)](#page-19-14) and [\(5\)](#page-4-1) to estimate  $Re<sub>L</sub>$  =  ${\rm Re}_\tau^4{\rm Re}^{-3}\hat{\phi}_{b,\rm max}^{-1},$ 

$$
Re_L = \frac{1}{\kappa} \frac{Re_{\tau}^4}{Re^3} \frac{27\alpha}{(2 - \mathcal{W}) \left[\frac{9}{\text{Pr}Re} + \frac{Re_{\tau}^2}{Re^2} (1 + \mathcal{W})^2\right]}, \quad (C12)
$$

and

$$
\lim_{\text{Re}\to\infty} \text{Re}_L = \frac{27\alpha \text{Re}_\tau^2}{4\kappa \text{Re}}.
$$
 (C13)

Using  $(C9)$ , this results in

$$
\text{Re}_{L} \sim \frac{27\alpha}{4\kappa} \frac{\text{Re}_{\tau}}{\ln(\text{Re}_{\tau})}.
$$
 (C14)

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