

# Two-fluid single-column modelling of Rayleigh-Bénard convection as a step towards multi-fluid modelling of atmospheric convection

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Multi-fluid models have recently been proposed as an approach to improving the representation of convection in weather and climate models. This is an attractive framework as it is fundamentally dynamical, removing some of the assumptions of mass-flux convection schemes which are invalid at current model resolutions. However, it is still not understood how best to close the multi-fluid equations for atmospheric convection. In this paper we develop a simple two-fluid, single-column model with one rising and one falling fluid. No further modelling of sub-filter variability is included. We then apply this model to Rayleigh-Bénard convection, showing that, with minimal closures, the correct scaling of the heat flux ( $Nu$ ) is predicted over six orders of magnitude of buoyancy forcing ( $Ra$ ). This suggests that even a very simple two-fluid model can accurately capture the dominant coherent overturning structures of convection.

**KEYWORDS**

convection, parametrization, turbulence, multi-fluid, Rayleigh-Bénard

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**Abbreviations:** CBL, convective boundary layer; DNS, direct numerical simulation; ISR, inertial sub range; LES, large-eddy simulation; NWP, numerical weather prediction; RBC, Rayleigh-Bénard convection.

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## 7 1 | INTRODUCTION

8 Despite being an important part of the global circulation and local variability, atmospheric convection is one of the  
9 weakest aspects of Numerical Weather Prediction (NWP) and climate models (Stephens et al., 2010; Sherwood et al.,  
10 2014; Stein et al., 2015; Clark et al., 2016). These difficulties are at least in part due to the “grey zone” problem:  
11 the resolution of current models is such that a typical grid spacing is neither much smaller, nor much larger, than a  
12 typical convective scale (say  $O(1\text{ km})$  for shallow convection), meaning that neither traditional parametrizations, nor  
13 so-called “explicit convection”, adequately represent the flow (Wyngaard, 2004; Holloway et al., 2014; Zhou et al.,  
14 2014; Clark et al., 2016). If a separation of scales exists between the clouds scale(s) and the grid spacing, simplifying  
15 assumptions may be made to aid in parametrization of sub-grid processes. In atmospheric convection, traditional clo-  
16 sures have assumed some form of balance between the large-scale forcing and the convective response, and that the  
17 area of a “grid box” taken up by cloud is small (Arakawa and Schubert, 1974; Plant, 2010). Both of these assumptions  
18 break down in the grey zone of current model resolutions, leading to unrealistic behaviour of models with traditional  
19 parametrizations.

20 At the other end of the scale, for grid spacings much smaller than the convective length scale(s), techniques of  
21 large-eddy simulation (LES) become applicable (see Mason, 1994, for a review). However, true LES requires very high  
22 resolution — typically  $O(10\text{ m})$  for the dry convective boundary layer (Sullivan and Patton, 2011) — which is beyond  
23 the computational capabilities of NWP and climate models for the foreseeable future. Many current operational  
24 forecasting models (e.g. the Met Office UKV configuration of the MetUM, DWD’s ICON-D2) use “explicit” convection,  
25 where the convection scheme is turned off. Some form of “turbulence” scheme is still required, often an LES-like eddy  
26 viscosity/diffusivity scheme. While these perform better at grey zone resolutions, there are still undesirable effects, in  
27 particular the prediction of incorrect length scales (cloud size and inter-cloud spacing) typically larger than observed  
28 scales, even in cases where the model *should* be able to resolve the smaller scale (Lean et al., 2008). There is thus both  
29 a need for parametrization well into the future, and a need for new parametrization approaches in the grey zone.

30 Multi-fluid modelling has recently been proposed as an approach to representing convection in the grey zone  
31 (Yano, 2014; Thuburn et al., 2018; Tan et al., 2018); similar equation sets are used for the modelling of multi-phase  
32 flows in engineering (e.g. Städtke, 2007). In the convection context, this takes inspiration from traditional mass-flux  
33 parametrizations in splitting the fluid into multiple components, which may represent updrafts, environment, down-  
34 drafts etc.. The split is applied directly to the governing equations, which are then spatially filtered, allowing a fully 3D  
35 and time-dependent framework to be derived (Thuburn et al., 2018; Shipley et al., 2021). Neither quasi-equilibrium  
36 nor small updraft fraction are assumed in the derivation. Each “fluid” evolves according to its own prognostic equa-  
37 tions, interacting with other fluids via the pressure gradient, and terms involving the exchange of mass, momentum,  
38 energy, and tracers. These exchange terms are the analogue of entrainment, detrainment, and cloud-base mass-flux  
39 in traditional models, and must be parametrized. Convection is inherently a part of the dynamics in this framework:  
40 there is no separate convection scheme which is called by the dynamical core.

41 The skewness of (joint) probability distribution functions of variables in convective flows is well known to be  
42 important (Larson et al., 2002; Zhu and Zuidema, 2009) and is often poorly treated in first or second-order turbulence  
43 closures; one approach to modelling this variability is assuming bi-Gaussian joint probability distributions in PDF-based  
44 convective closures (Larson et al., 2012; Fitch, 2019). Each Gaussian can be thought of as a different component of  
45 the fluid. A potential advantage of the multi-fluid approach is that even the simplest possible multi-fluid model, a two  
46 fluid model, intrinsically captures information about odd-order moments. It is therefore possible that the multi-fluid  
47 method can provide a better low-order approximation for flows with bimodal distributions, or large skewness.

48 In order to build a multi-fluid model of atmospheric convection, the multi-fluid equation set must be closed. The

49 form of these closures directly depends on the definition of the fluid partitions (de Rooy et al., 2012; Shipley et al.,  
50 2021). For example, the single-column 2-fluid model of Thuburn et al. (2019) contains entrainment and detrainment  
51 closures designed to capture coherent structures in the convective boundary layer, whereas the closures in Cohen  
52 et al. (2020) are designed to model a second fluid in the cloud layer only. Perturbation pressure closures for the latter  
53 approach were suggested in He et al. (2020). Entrainment and detrainment closures based on velocity divergence, and  
54 a bulk viscous parametrization for the perturbation pressure, were proposed and tested in Weller et al. (2020), but  
55 the test cases used for comparison were non-turbulent, unlike the real atmosphere. All of these multi-fluid models  
56 have been single-column, and used standard atmospheric test cases (e.g. dry rising bubble, dry convective boundary  
57 layer, oceanic and continental shallow cumulus, diurnal deep convection) for verification. While prior work shows the  
58 considerable promise of the multi-fluid method, little work has been done testing the response of a specific multi-  
59 fluid scheme to a variety of forcings, or suggested how the closure constants should scale with that forcing. Such  
60 investigation could lead to more consistent results compared to tuning a model to a handful of test cases.

61 To gain a better understanding of the multi-fluid equations, and how some of the new closure terms affect the  
62 solution, we present a single-column model of dry Rayleigh-Bénard convection (RBC) with one rising and one falling  
63 fluid. RBC is the simplest relevant convection problem: the equations and boundary conditions are as simple as  
64 possible while still allowing for a fully turbulent convective solution. RBC has been extensively studied, and a wealth  
65 of experimental, numerical, and theoretical results make it a well-constrained starting point (Chandrasekhar, 1961;  
66 Ahlers et al., 2009; Chillà and Schumacher, 2012). In particular, the scaling of bulk buoyancy and momentum transport  
67 with the applied buoyancy forcing is well understood over at least ten orders of magnitude.

68 It is important to understand the response of the model in a fully-parametrized equilibrium setting before moving  
69 to the grey zone. This will help pin down the physics of a multi-fluid model of convection, free of the complexities –  
70 especially microphysics and phase changes – of the real atmosphere.

71 The paper begins with an overview of Rayleigh-Bénard convection in section 2, motivating its use as a reasonable  
72 testbed for developing insights into “real-world” convection. Results from 2D direct numerical simulations (DNS) of  
73 dry RBC are presented, and shown to agree with reference results. In section 3 a multi-fluid Boussinesq equation  
74 set is presented, along with a discussion of how and why this equation set differs from previous papers on multi-  
75 fluid convection parametrization. Closures for one rising and one falling fluid which attempt to capture the large-  
76 scale overturning circulation are presented in section 3.1, and a scaling argument is presented for the magnitude  
77 of the pressure differences between the fluids. The numerical method is then described in section 4. In section 5,  
78 results of the two-fluid single-column model (section 3.1) are compared with horizontally-averaged results from the  
79 DNS (section 2.1) over a range of buoyancy forcing spanning seven orders of magnitude ( $10^3 \leq Ra \leq 10^{10}$ ), and  
80 the sensitivity of the model to its two dimensionless closure constants is investigated. The paper concludes with a  
81 summary of its results and their relevance to convection parametrizations, and a discussion of avenues for future  
82 research.

## 83 2 | RAYLEIGH-BÉNARD CONVECTION (RBC)

84 The Rayleigh-Bénard problem is the simplest fluid dynamical model of convection. First studied experimentally by  
85 Bénard (1900), the problem was given a theoretical treatment by Rayleigh (1916) which has been the basis of over a  
86 century of investigation. Rayleigh (1916) studied the motion of a Boussinesq fluid confined between two perfectly con-  
87 ducting horizontal plates of infinite extent, each held at a constant uniform temperature. For mathematical tractability  
88 he considered stress-free velocity boundary conditions at the plates; the no-slip case was tackled by Jeffreys (1926,

1928). RBC has long been of interest to the meteorological community, being the basis of the Lorenz (1963) seminal discovery of deterministic chaos, and a key component of our understanding of convective systems (Emanuel, 1994, ch. 3). Moist extensions of the model have been considered to gain insight into moist convection, though far less work has been performed on moist versions of the problem than on the dry case (Bretherton, 1987, 1988; Pauluis and Schumacher, 2010; Weidauer and Schumacher, 2012; Vallis et al., 2019). In this section, the classical results relevant to this paper are collected. The canonical text covering stability and the onset of convection is Chandrasekhar (1961); recent reviews covering fully turbulent convection are Ahlers et al. (2009); Chillà and Schumacher (2012).

The setup of the Rayleigh-Bénard problem is as follows. A Boussinesq fluid is confined between two smooth, flat, horizontal plates, a fixed distance  $H$  apart. Each of these is held at a fixed buoyancy,  $\pm \Delta B/2$ , with no-slip, no-normal flow velocity boundary conditions. For both analytical and numerical simplicity we choose the lateral boundaries to be periodic in all fields. The motion of the fluid is described by the following Boussinesq equations of motion:

$$\frac{D\mathbf{u}}{Dt} = b\mathbf{k} - \nabla P + \nu \nabla^2 \mathbf{u}, \quad (1)$$

$$\frac{Db}{Dt} = \kappa \nabla^2 b, \quad (2)$$

$$\nabla \cdot \mathbf{u} = 0. \quad (3)$$

Here  $\mathbf{u}$  denotes the velocity field of the fluid;  $b := g(\rho_{\text{ref}} - \rho)/\rho_{\text{ref}}$  its buoyancy<sup>1</sup>;  $P := p/\rho_{\text{ref}}$  its pressure potential;  $\nu$  its kinematic viscosity;  $\kappa$  its buoyancy diffusivity; and  $\mathbf{k}$  is a unit vector antiparallel to gravity, defining the vertical ( $z$ ) direction. All variables are defined relative to a resting, uniformly constant-density, hydrostatically-balanced pressure reference state.

A diffusive nondimensionalization of equations (1)-(3) by the external parameters,  $\hat{\mathbf{x}} := \mathbf{x}/H$ ,  $\hat{b} := b/\Delta B$ ,  $\hat{t} := t\kappa/H^2$ ,  $\hat{\mathbf{u}} := \mathbf{u}H/\kappa$ ,  $\hat{P} := H^2/\kappa\nu$  (as Chandrasekhar, 1961; Emanuel, 1994, but choosing a diffusive rather than viscous time-scale), shows that two dimensionless parameters govern the flow (the boundary conditions are given for completeness):

$$\frac{D\hat{\mathbf{u}}}{D\hat{t}} = \text{Pr} \left( \text{Ra} \hat{b}\mathbf{k} - \hat{\nabla} \hat{P} + \hat{\nabla}^2 \hat{\mathbf{u}} \right), \quad (4)$$

$$\frac{D\hat{b}}{D\hat{t}} = \hat{\nabla}^2 \hat{b}, \quad (5)$$

$$\hat{\nabla} \cdot \hat{\mathbf{u}} = 0, \quad (6)$$

$$\hat{b}(\hat{z} = 0) = \frac{1}{2}, \quad \hat{b}(\hat{z} = 1) = -\frac{1}{2}, \quad (7)$$

$$\hat{\mathbf{u}}(\hat{z} = 0, 1) = \mathbf{0}. \quad (8)$$

Nondimensionalized variables are denoted by a hat, and the dimensionless parameters are defined by:

$$\text{Ra} := \frac{\Delta B \cdot H^3}{\kappa \nu}, \quad \text{Pr} := \frac{\nu}{\kappa}. \quad (9)$$

The Rayleigh number, Ra, is the ratio of buoyancy forcing ( $\Delta B$ ) to viscous diffusion ( $\kappa\nu/H^3$ ); and the Prandtl number, Pr, is the ratio of the diffusion of momentum ( $\nu$ ) to the diffusion of buoyancy ( $\kappa$ ). The former can thus be seen as mea-

<sup>1</sup>For our desired application to atmospheric convection,  $(\rho_{\text{ref}} - \rho)/\rho_{\text{ref}} \simeq (\theta - \theta_{\text{ref}})/\theta_{\text{ref}}$ , where  $\theta$  is the potential temperature, though much previous work on Rayleigh-Bénard convection (RBC) is performed in terms of temperature, using the approximation  $(\rho_{\text{ref}} - \rho)/\rho_{\text{ref}} \simeq (T - T_{\text{ref}})/T_{\text{ref}}$ . The equation set retains the same form.

123 sure of the applied forcing in RBC, whereas the latter is an intrinsic property of the fluid. This nondimensionalization  
 124 shows that any two RBC systems with the same Ra and Pr support the same solutions, i.e. are self-similar.<sup>2</sup>

125 It is worth noting that this nondimensionalization specifically singles out the diffusive regime as the regime of  
 126 interest, relevant for considerations of stability. For consideration of the convective solutions, a nondimensionalization  
 127 based on the buoyancy forcing is more useful. This “free fall” or “free convective” scaling gives velocity and time scales  
 128  $U_B := \sqrt{\Delta B H}$ ,  $T_B := \sqrt{H/\Delta B}$ , and is ubiquitous in the CBL literature (where  $U_B$  is denoted  $w^*$ , see, e.g., Garratt (1994)).  
 129 Such a scaling also gives an a priori estimate for the Reynolds number,  $\text{Re} \propto \text{Ra}^{1/2} \text{Pr}^{-1/2}$ .<sup>3</sup> This approximate Re (Ra)  
 130 scaling is observed for the regimes applicable to this paper.

131 The equation set (4)-(8) has a unique stationary zero-flow solution, with a linear buoyancy gradient between the  
 132 plates and a quadratic pressure profile:

$$133 \quad \mathbf{u} = \mathbf{0}, \quad b = \frac{1}{2}(1-z), \quad P = P_0 + \frac{z}{2}\left(1 - \frac{z}{2}\right). \quad (10)$$

135 This solution is both linearly and nonlinearly unstable to perturbations if and only if the Rayleigh number exceeds a  
 136 critical value,  $\text{Ra}_c$ ; importantly, the stability does not depend on the Prandtl number (see, for instance, Chandrasekhar,  
 137 1961; Joseph, 1966; Lindsay and Straughan, 1990). Below  $\text{Ra}_c$ , solutions are purely diffusive; above  $\text{Ra}_c$ , a circulation  
 138 develops which increases the heat transport. This circulation can either be steady, periodic, quasi-periodic, or turbu-  
 139 lent, depending on the governing parameters (Ra, Pr). The precise value of  $\text{Ra}_c$  depends on the velocity boundary  
 140 conditions at the top and bottom boundaries, but not on the dimensionality of the domain; for our chosen no-slip  
 141 conditions,  $\text{Ra}_c \approx 1708$ , and the wavelength of the most unstable mode is  $\lambda_c \approx 2.02H$  (Chandrasekhar, 1961, table 3).

142 The domain- and time-averaged dimensionless buoyancy flux is given by the Nusselt number:

$$143 \quad \text{Nu} := \left\langle \mathbf{k} \cdot (\hat{\mathbf{u}}\hat{b} - \hat{\nabla}\hat{b}) \right\rangle_{V,t} = \left\langle \hat{w}\hat{b} - \frac{\partial\hat{b}}{\partial z} \right\rangle_{A,t}, \quad (11)$$

145 which is the ratio of the actual buoyancy flux to the buoyancy flux of the purely diffusive solution. Averaging the  
 146 buoyancy equation (5) over a horizontal plane and over time (denoted  $\langle \dots \rangle_{A,t}$ ) shows that the Nusselt number is  
 147 independent of height in a statistically stationary flow.

148 Exact results for the domain- and time-averaged kinetic and thermal dissipation rates,  $\varepsilon_u$  and  $\varepsilon_b$ , are given by  
 149 (Siggia, 1994; Chandrasekhar, 1961, appendix 1):

$$150 \quad \varepsilon_u := \langle \nabla \mathbf{u} : \nabla \mathbf{u} \rangle_{V,t} = \text{Ra}(\text{Nu} - 1), \quad (12)$$

$$151 \quad \varepsilon_b := \langle \nabla b \cdot \nabla b \rangle_{V,t} = \text{Nu}. \quad (13)$$

153 Here the “double dot product” denotes the complete contraction of two rank-two tensors, following the convention  
 154  $\mathbf{A} : \mathbf{B} := \sum_{a,b} A_{ab} B^{ab}$ . Thus the vertical buoyancy flux is the only quantity that characterizes the stationary-state global  
 155 energetic response of the system to the applied forcing (Ra, Pr)<sup>4</sup>. The statistically steady-state Rayleigh-Bénard prob-  
 156 lem can then be framed as asking the question: if we apply a buoyancy forcing Ra to a Boussinesq fluid characterized

<sup>2</sup>A third parameter, the aspect ratio of the domain,  $\Gamma := L/H$ , enters via the lateral boundary conditions; however, the dependence upon the aspect ratio is generally weak so long as  $\Gamma > 1$  – see Ahlers et al. (2009), section 3E; also Johnston and Doering (2009); Bailon-Cuba et al. (2010); Zhou et al. (2012) – and the dependence is weaker for periodic boundaries than for rigid boundaries.

<sup>3</sup>The a priori scaling for the Nusselt number that this predicts,  $\text{Nu} \propto \text{Ra}^{1/2}$  – the so-called “ultimate scaling” – is steeper than observed to date in experimental or numerical dry RBC, because the non-turbulent surface layers next to the boundaries prevent a thermal shortcut.

<sup>4</sup>It is worth noting that these results (12)-(13) are quite general; in particular they do not rely on the plates being smooth and flat, and they apply equally well also to the cases of stress-free velocity or constant buoyancy flux boundary conditions.

157 by Pr, what is the resulting Nu? Scaling theories for Nu as a function of Ra and Pr are well-developed, and there is  
 158 good agreement between the theory and numerical and experimental results until at least  $Ra = 10^{11}$  for  $Pr = O(1)$   
 159 (Ahlers et al., 2009; Chillà and Schumacher, 2012). It is therefore a strong test of any dynamical low-order model of  
 160 RBC to reproduce these scalings.

## 161 2.1 | 2D direct numerical simulation of RBC

162 To provide a reference “truth” for later sections in the paper, results from two dimensional direct numerical simulations  
 163 of Rayleigh-Bénard convection over a wide range of Ra are presented. These simulations also serve to illustrate the  
 164 phenomenology of RBC, and to indirectly validate the numerical methods via comparison with reference results.

165 While the restriction to two dimensions may seem like too great a simplification, global and large-scale results of  
 166 Rayleigh-Bénard convection in two and three dimensions are remarkably similar so long as the Prandtl number is not  
 167 too small. The classical results regarding the critical Rayleigh number, critical wavelength, and onset of convection  
 168 are unaffected (see (Chandrasekhar, 1961, ch. 2); though not explicitly stated, the stability analysis does not depend  
 169 on the dimensionality of the domain). After the onset of convection, for  $O(1)$  Pr and greater, the scalings of global  
 170 parameters such as the Nusselt and Reynolds numbers, as well as the boundary layer depths, are virtually the same  
 171 in 2D as in 3D (although the magnitudes differ slightly) — see Schmalzl et al. (2004). Many theoretical analyses of  
 172 the problem have either included two dimensions as a special case, or actually assumed only two dimensions, the  
 173 successful Grossmann and Lohse (2000) scaling theory for the Nusselt and Rayleigh numbers being a prime example  
 174 of the latter. Therefore we choose to perform 2D simulations, given the similarity between 2D and 3D results and  
 175 the vastly reduced computational requirements for 2D calculations.

176 Our simulation suite runs from fully diffusive ( $Ra \approx 10^2$ ) to well into the turbulent regime ( $Ra \approx 10^{10}$ ). Rayleigh  
 177 numbers have been chosen such that there is at least one simulation per factor of ten of Ra, with extra simulations  
 178 run in the vicinity of  $Ra_c$ . The Prandtl number is fixed to be  $Pr = 0.707$ , the value for dry air at STP. Reviews of RBC  
 179 suggest that qualitative results remain similar so long as the asymptotic range of Pr is the same, i.e.  $Pr = O(1)$  rather  
 180 than  $Pr \rightarrow 0$  or  $\infty$  (Ahlers et al., 2009; Chillà and Schumacher, 2012). In particular, the scaling exponent  $Nu \propto Ra^\beta$   
 181 is not strongly Prandtl-number dependent.

### 182 2.1.1 | Choice of resolution

- 183 • By “resolution”,  $\Delta_r$ , we mean the smallest length scale at which structures of the flow are well captured by the  
 184 model.
- 185 • By “filter scale”,  $\Delta_f$ , we mean the length scale(s) associated with any filter applied to the flow, whether to the  
 186 solutions or to the governing equations.
- 187 • By “grid scale” (alternatively, “grid length” or “grid spacing”),  $\Delta_g$ , we mean the actual distance between points (or  
 188 cell centres) within a discretized model.

189 A direct numerical simulation of a fluid (“DNS”) must “resolve” all dynamically relevant scales of the fluid flow in order  
 190 to justify the assumption that no small-scale processes need to be parametrized. But there are various metrics by  
 191 which we can test whether a flow is “resolved”. To *fully* resolve a turbulent flow, the grid spacing must resolve at least  
 192 a factor of ten into the viscous subrange (Kerr, 1985), which is very computationally expensive. However, to get the  
 193 majority of the statistics right the requirements are less extreme: the Kolmogorov dissipation length,  $\eta := H(Pr^2/\epsilon_u)^{1/4}$ ,  
 194 must be resolved (Grötzbach, 1983). Within fully-developed turbulence in the bulk of the fluid the exact result for

195 the global kinetic energy dissipation rate, (12), may be used to estimate the smallest dynamically relevant scale:

$$196 \quad \frac{\eta}{H} = \left( \frac{\text{Pr}^2}{(\text{Nu}-1) \text{Ra}} \right)^{\frac{1}{4}}. \quad (14)$$

198 Towards the boundaries, the kinetic and thermal boundary layers must be resolved – dissipation is typically higher  
 199 in these regions, reducing the smallest dynamically relevant length scale. Shishkina et al. (2010) estimated local dis-  
 200 sipation lengths based on dissipation rates defined within the boundary layers, using these to estimate the minimum  
 201 number of points  $N_u, N_b$  required within each boundary layer (thickness  $\delta_u, \delta_b$ ) in order to adequately resolve the  
 202 flow. This estimate is for  $10^6 < \text{Ra} < 10^{10}$ , so for  $\text{Ra} \leq 10^6$  we use the values of  $N_u, N_b$  estimated for  $\text{Ra} = 10^6$ . Note  
 203 that this extra resolution is only required in the vertical direction.

204 At any point in the flow the smallest of  $\{\eta, \delta_b/N_b, \delta_u/N_u\}$  must be resolved. Collecting the results of Grötzbach  
 205 (1983) and Shishkina et al. (2010), the grid spacing is required to satisfy  $\Delta x_\eta < 2\eta, \Delta x_b < \delta_b / 0.35 \text{Ra}^{0.15}, \Delta x_u <$   
 206  $\delta_u / 0.31 \text{Ra}^{0.15}$  to be adequate to resolve each respective scale.

207 To make use of the resolution requirements, the boundary layer thicknesses must be estimated. Since the centre  
 208 of the domain will be statistically well-mixed after the onset of convection, we must have  $\delta_b/H \sim 1/2 \text{Nu}$ . For the  
 209 parameter regimes of this study,  $\text{Nu} \sim \text{Ra}^{2/7}$  and so  $\delta_b/H \sim \text{Ra}^{-2/7}$  (Castaing et al., 1989; Shraiman and Siggia, 1990;  
 210 Ahlers et al., 2009). Prandtl-Blasius boundary layer theory suggests that the kinetic boundary layer thickness should  
 211 scale as  $\delta_u/H \sim \text{Ra}^{-1/4}$ , and  $\delta_u < \delta_b$  is expected over the entire Rayleigh number range here considered (Ahlers et al.,  
 212 2009, fig. 3). To estimate the prefactors, an over-resolved simulation with  $\Delta x/H = \Delta z/H = 0.01$  was run at  $\text{Ra} = 10^5$ ,  
 213 finding  $\delta_u \approx 0.56 \text{Ra}^{-1/4}, \delta_b \approx 2.8 \text{Ra}^{-2/7}$ ; these prefactors do indeed ensure that  $\delta_u < \delta_b$  for the Rayleigh number  
 214 regime of the study.

215 For each  $\text{Ra}$  we construct an orthogonal, rectangular grid such that the grid spacing is always smaller than the  
 216 smallest of these length scales. This grid consists of, in the  $z$ -direction: a uniform grid with spacing  $\Delta z^{(0)} = \Delta x_u$  for  
 217  $0 \leq |z - z_{\text{boundary}}| \leq \delta_u$ ; a uniform grid with spacing  $\Delta z^{(1)} : \Delta x_u < \Delta z^{(1)} < \Delta x_b$  for  $\delta_u < |z - z_{\text{boundary}}| \leq \delta_b$ ; a  
 218 nonuniform grid expanding linearly from  $\Delta z^{(1)} \rightarrow \Delta z^{(2)}$  over the range  $\delta_b < |z - z_{\text{boundary}}| \leq 2\delta_b$ ; a uniform grid  
 219 with spacing  $\Delta z^{(2)} = 2\eta$  for  $2\delta_b < z < H - 2\delta_b$ . In the horizontal direction, grid spacing is uniformly equal to  $2\eta$   
 220 throughout the domain. Details of the grid for each simulation are given in table 1.

221 In principle, we could directly check that the resolution is sufficient post-hoc by refining the grid and re-computing  
 222 all of the statistics; if they do not change as the resolution increases, then the lower resolution “fully resolves” the  
 223 flow. In practice, for this paper we note that the grid spacings of our simulations are comparable to those in similar  
 224 DNS of 2D RBC (e.g. Johnston and Doering, 2009). Details of the numerical method are given in section 4 as a special  
 225 case of the multi-fluid solver.

## 226 2.1.2 | Calculation of Nu, Re, $\delta_b$

227 The Nusselt number, Reynolds number, and boundary layer depths are calculated as follows:

228 Nu: The most direct way of calculating Nu is to integrate the (dimensionless) heat flux over the entire domain,  
 229 then take a time average:  $\text{Nu} = \langle wb - \partial b / \partial z \rangle_{V,t}$ . However, if the flow is statistically stationary, then the  
 230 time-averaged *horizontally averaged* (dimensionless) heat flux is independent of height, so calculating the time-  
 231 averaged vertical buoyancy gradient averaged over the top and bottom boundaries gives a second estimate,  
 232  $\text{Nu}_w := \langle -\partial b / \partial z \rangle_{A,t; z=0,H}$ . The equivalence of these two expressions for Nu provides an extra check for the



Ra	$T_{\text{tot}}/4T_B$	$\Delta t/4T_B$	$\Delta z_c/H = \Delta x/H$	$\Delta z_w/H$	$\eta/H$	$\delta_u/H$
$10^2$	25	$6.393 \times 10^{-5}$	0.04	0.04	N/A	N/A
$10^3$	25	$1.599 \times 10^{-3}$	0.04	0.04	N/A	N/A
$1.6 \times 10^3$	51	$6.393 \times 10^{-4}$	0.02	0.02	N/A	N/A
$1.7 \times 10^3$	51	$6.393 \times 10^{-4}$	0.02	0.02	N/A	N/A
$1.8 \times 10^3$	127	$6.393 \times 10^{-4}$	0.02	0.02	N/A	N/A
$2 \times 10^3$	38	$7.992 \times 10^{-4}$	0.02	0.02	$1.410 \times 10^{-1}$	$8.459 \times 10^{-2}$
$10^4$	25	$1.598 \times 10^{-3}$	0.02	0.01	$7.494 \times 10^{-2}$	$5.656 \times 10^{-2}$
$5 \times 10^4$	25	$1.998 \times 10^{-3}$	0.02	0.01	$4.240 \times 10^{-2}$	$3.783 \times 10^{-2}$
$10^5$	38	$1.598 \times 10^{-3}$	0.02	0.01	$3.346 \times 10^{-2}$	$3.181 \times 10^{-2}$
$5 \times 10^5$	25	$9.990 \times 10^{-4}$	0.02	$7.067 \times 10^{-3}$	$1.951 \times 10^{-2}$	$2.127 \times 10^{-2}$
$10^6$	25	$9.990 \times 10^{-4}$	0.02	$5.963 \times 10^{-3}$	$1.551 \times 10^{-2}$	$1.789 \times 10^{-2}$
$5 \times 10^6$	38	$9.990 \times 10^{-4}$	$1.797 \times 10^{-2}$	$2.990 \times 10^{-3}$	$9.151 \times 10^{-3}$	$1.196 \times 10^{-2}$
$10^7$	60	$5.115 \times 10^{-4}$	$1.454 \times 10^{-2}$	$2.515 \times 10^{-3}$	$7.300 \times 10^{-3}$	$1.006 \times 10^{-2}$
$2 \times 10^7$	51	$3.996 \times 10^{-4}$	$1.165 \times 10^{-2}$	$2.114 \times 10^{-3}$	$5.827 \times 10^{-3}$	$8.459 \times 10^{-3}$
$10^8$	38	$3.197 \times 10^{-4}$	$6.729 \times 10^{-4}$	$1.130 \times 10^{-3}$	$3.459 \times 10^{-3}$	$5.657 \times 10^{-3}$
$10^9$	22 (45)	$1.279 \times 10^{-4}$	$4.543 \times 10^{-4}$	$4.544 \times 10^{-4}$	$1.645 \times 10^{-3}$	$3.181 \times 10^{-3}$
$10^{10}$	20 (76)	$7.992 \times 10^{-5}$	$1.563 \times 10^{-3}$	$1.789 \times 10^{-4}$	$7.832 \times 10^{-4}$	$1.789 \times 10^{-3}$

TABLE 1 Details of grid spacing, time-step size, and simulation time for the 2D DNS of RBC (section 2.1).

Times are nondimensionalized by the (approximate) eddy turnover time,  $T_e \approx 4\sqrt{H/\Delta B}$ . The final two columns give the physical length scales used to estimate the required resolution, the (bulk) Kolmogorov dissipation length  $\eta/H$  (equation (14)) and the kinetic boundary layer thickness,  $\delta_u/H \approx 0.56 \text{Ra}^{-1/4}$ . The  $\text{Ra} = 10^9$  and  $10^{10}$  simulations were spun up on a coarser grid (the  $\text{Ra} = 10^8$  grid), then after reaching equilibrium the grid was refined. The simulation time on the finer grid is given, followed by, in parentheses, the total simulation time on both grids for that Rayleigh number.

233 statistical steadiness of the numerical solutions. Another check for statistical stationarity is provided via the kinetic and thermal dissipation rates (calculated using equations (12)-(13)). Thus for a statistically stationary state, convergence of  $\text{Nu} = \text{Nu}_w = \varepsilon_b = 1 + \varepsilon_u/\text{Ra}$  is required.

236 Re: The calculation of a Reynolds number based on the definition  $\text{Re} := UL/\nu$  requires the choice of a velocity scale and a length scale. For RBC, the only length scale we can reasonably choose for a bulk Reynolds number must be the domain height  $H$ , as this is the only external length scale in the problem. However, what is a reasonable representative velocity scale,  $U$ ? Several possible choices are suggested in Kerr (1996); Ahlers et al. (2009); we shall consider velocity scales based on the turning points of the velocity variance profile:

241 
$$U_1 := \sqrt{\text{mean}(\text{var}(u)_{x,t})}; \quad U_2 := \sqrt{\text{max}(\text{var}(u)_{x,t})}; \quad U_3 := \sqrt{\text{max}(\text{var}(w)_{x,t})} \quad (15)$$

243 An a priori estimate of  $\text{Re}$  can be found by assuming free-convective scaling,  $U = U_B := \sqrt{\Delta B H}$ , implying  $\text{Re} =$

$$\sqrt{\Delta B H^3 / \nu^2} = \text{Ra}^{1/2} \text{Pr}^{-1/2}.$$

$\delta_b$ : If the flow is statistically stationary, the buoyancy will be well-mixed in the interior of the domain, the time-averaged buoyancy profile must be approximately constant outside of the boundary layers, and approximately linear within due to the fixed buoyancy boundary conditions. Thus one measure of the thermal boundary layer thickness is

$$\delta_b^{(1)} := -\frac{\Delta B}{2 \frac{d\langle b \rangle_{x,t}}{dz} |_{\text{wall}}}. \quad (16)$$

Following Kerr (1996), we also estimate the thermal boundary layer thickness from the locations of the maxima of the buoyancy variance profile:

$$\delta_b^{(2)} := |z(\max(\text{var}(b)_{x,t})) - z(\text{wall})|. \quad (17)$$

Both the upper and lower boundary layer thicknesses should be the same.

The above time averages are calculated over at least 5 eddy turnover times ( $T_e \approx 4 T_B$ ). Time-averages are also calculated over twice and three times this minimum averaging time, and all simulations show convergence between the averages taken over these three different times. The total simulation time for each Rayleigh number is given in table 1.

## 2.2 | The relevance of RBC to atmospheric flows

While RBC is a valuable test problem in its own right, it is worth considering similarities with and differences from atmospheric flows, in particular the dry atmospheric convective boundary layer (CBL).

Besides the complexities of moisture, the dry RBC problem differs from even dry atmospheric convection in a few important ways. Firstly, the Boussinesq approximation is of questionable validity even on the scale of the atmospheric boundary layer; in practice however, it has long been used in the LES community with excellent results (Sullivan and Patton, 2011, e.g. ). Furthermore, the Boussinesq form has been used to facilitate analysis; experiments using a non-Boussinesq (fully compressible) version of the same code show little qualitative or quantitative differences from their Boussinesq counterparts.

Secondly, the lower boundary in the CBL is neither smooth, nor uniformly heated. Recent results show that neither nonuniform heating (Bakhuis et al., 2018) nor rough boundaries (Zhu et al., 2019; Toppaladoddi et al., 2021) drastically change the dynamics of RBC, though the latter does tend to increase the heat flux towards the so-called “ultimate regime”, equivalent to the free-convective regime which dominates discussion of scaling in the atmospheric convective boundary layer.

Thirdly, the fixed buoyancy boundary conditions are quite different to CBL conditions, where the lower boundary is closer to (and is often modelled as) a fixed buoyancy flux, and there is no fixed upper boundary for the convection (instead there is a stable atmospheric layer). In practice, solutions of RBC with fixed flux vs. fixed value boundary conditions are similar, especially in 2D (Verzicco and Sreenivasan, 2008; Johnston and Doering, 2009) (as are LES simulations of the CBL). It is thus only the upper boundary that introduces a major difference between RBC and the CBL. Even in that case there has been recent progress on studying modified Rayleigh-Bénard convection with the compensating heat flux provided by radiation in a layer of finite thickness (Lepot et al., 2018; Doering, 2019), which

279 the first authors note “spontaneously achieves the ‘ultimate’ regime of thermal convection”.

280 We thus consider the classical Rayleigh-Bénard problem to be sufficiently close to atmospheric convection to  
 281 provide a reasonable testbed for investigating the behaviour of a multi-fluid model of turbulent convection. There  
 282 remains the question of the applicable parameter regime, discussed in the next section.

### 283 2.2.1 | An analogy between constant-viscosity RBC and large-eddy simulation of higher- 284 Ra RBC.

285 Atmospheric flows generally involve very high Reynolds number; for example, the CBL might have depth  $\approx 1000$  m, and  
 286 (even without a mean wind) velocities in convective updraughts  $\approx 1 \text{ m s}^{-1}$ . With kinematic viscosity of air  $\approx 10^{-5} \text{ m}^2 \text{ s}^{-1}$   
 287 we have  $\text{Re} \approx 10^8$ . In the context of RBC, this would lead to  $\text{Ra} \approx 10^{16}$ , i.e. much larger than in our simulations.  
 288 Given the above considerations of resolution, a DNS of this problem is computationally impossible in 3D with current  
 289 computing power and would be a challenge even in 2D.

290 The atmospheric science community address this problem using Large-Eddy Simulation (LES) as reviewed by  
 291 Mason (1994). LES is based upon spatially low-pass filtering the equations of motion with a filter with characteristic  
 292 scale  $\Delta_f$  chosen such that the unfiltered flow remains well within the self-similar Kolmogorov inertial sub-range (ISR)  
 293 of scales. In this case, the sub-filter contribution to turbulent fluxes is small and can be represented by a simple  
 294 eddy-viscosity. In practice, the eddy-viscosity proposed by Smagorinsky (1963) has been found to give good results  
 295 provided the simulation actually is well within the ISR.

296 In fact, Mason (1994) points out that acceptable results are obtained from a simulation of the CBL in which a  
 297 constant viscosity is used at each level based upon the horizontal average of the Smagorinsky value. One might go  
 298 further and suggest that the height-dependence is required primarily close to the surface and boundary-layer top  
 299 where eddy length-scales are restricted. In this case, a simple view of LES is as follows. With a well-developed ISR  
 300 the flow is essentially independent of  $\text{Re}$ . For sufficiently large  $\text{Re}$  we can choose an artificial larger viscosity such that  
 301 the range of scales in the flow is smaller as the Kolmogorov microscale (i.e. the eddy scale at which  $\text{Re} = 1$ ) is larger.  
 302 The turbulent kinetic energy dissipation rate ( $\varepsilon$ ) remains the same as does the flow at larger scales. Essentially the  
 303 same argument applies to use of wind-tunnels with scale models.

304 Smagorinsky provides us with a method to estimate this artificially large viscosity, but let us take a more basic  
 305 view. In the ISR the energy spectrum  $E(k) = K_0 \varepsilon^{\frac{2}{3}} k^{-\frac{5}{3}}$ , with  $K_0$  a constant and  $k$  the wave number. Suppose we  
 306 choose a filter scale with wave number  $k_f$ , then the “turbulent” kinetic energy (TKE) in the subfilter flow has a velocity  
 307 scale  $U_f$  given by

$$308 \quad U_f^2 = \int_{k_f}^{\infty} E(k) dk = \frac{2}{3} K_0 \varepsilon^{\frac{2}{3}} k_f^{-\frac{2}{3}} \quad (18)$$

309 Prandtl argues, by analogy with the kinetic theory of gases, that the eddy diffusivity is a product of the turbulent  
 310 velocity scale and the “mean free path” or “mixing length”. It is possible to show this more rigorously using the dynam-  
 311 ical equation for stress. We assume that the mixing length scales with  $k_f^{-1}$  and hence the eddy viscosity is given by  
 312  $\nu_f \propto U_f k_f^{-1}$ . This assumption is precisely the same as stating that the eddy Reynolds number,  $\text{Re}_f \equiv U_f k_f^{-1} / \nu_f \approx 1$ , i.e.  
 313 the filter scale is proportional to the Kolmogorov microscale of the filtered flow,  $\eta_f \propto k_f^{-1}$ . Indeed, if we absorb the  
 314 constants in eq. (18) into  $\eta_f$ , the Kolmogorov microscale for the filter, then  $U_f = \varepsilon^{\frac{1}{3}} \eta_f^{\frac{1}{3}}$ ,  $\text{Re}_f \equiv U_f \eta_f / \nu_f = 1$  and all of  
 315 the Kolmogorov scales apply.

316 Note that with this viscosity the kinematic deviatoric stress is given by  $\boldsymbol{\tau} = U_f \eta_f (\nabla \mathbf{u} + \nabla \mathbf{u}^T)$ . The spatially

317 filtered equation for the TKE, in steady state and ignoring the transport term (both assumptions being appropriate for  
 318 the homogeneous isotropic turbulence the ISR is considered to represent) leads to a simple balance between shear  
 319 production and dissipation:

$$320 \quad \boldsymbol{\tau} : (\nabla \mathbf{u} + \nabla \mathbf{u}^T) = 2\varepsilon \quad (19)$$

321 The TKE is given by  $\frac{1}{2}U_f^2$ . The scaling above gives  $\varepsilon = U_f^3/\eta_f$  (so the timescale for dissipation is  $\eta_f/(2U_f)$ ) then this  
 322 balance becomes:

$$323 \quad U_f \eta_f (\nabla \mathbf{u} + \nabla \mathbf{u}^T) : (\nabla \mathbf{u} + \nabla \mathbf{u}^T) = 2 \frac{U_f^3}{\eta_f} \quad (20)$$

324 from which  $U_f = \eta_f \left[ \frac{1}{2} (\nabla \mathbf{u} + \nabla \mathbf{u}^T) : (\nabla \mathbf{u} + \nabla \mathbf{u}^T) \right]^{\frac{1}{2}}$ , leading to the Smagorinsky (1963) formulation of viscosity.

325 To give a simple example, suppose we have a convective boundary layer with  $H$  the depth of the layer, say 1000  
 326 m and convective velocity scale  $U = 2 \text{ m s}^{-1}$ , corresponding to  $\Delta B \approx 4 \times 10^{-3} \text{ m s}^{-2}$ . Then  $\text{Re} = UH/\nu = 1.33 \times 10^8$   
 327 and  $\text{Ra} = 1.8 \times 10^{16}$ . The ‘‘outer’’ mixing length is often taken to be  $L = 0.15H$ . Then a crude estimate of  $\varepsilon$  is  
 328  $\varepsilon = U^3/L = 8/150 \text{ m}^2 \text{ s}^{-3} = 5.3 \times 10^{-2} \text{ m}^2 \text{ s}^{-3}$ . The Kolmogorov microscale is thus  $\eta = (\nu^3/\varepsilon)^{\frac{1}{4}} \approx 0.5 \text{ mm}$ . If we choose  
 329 a filter scale such that  $\eta_f = 1 \text{ m}$ , then  $U_f = 0.376 \text{ m s}^{-1}$ , the eddy viscosity is  $0.376 \text{ m}^2 \text{ s}^{-1}$  and the Reynolds number of  
 330 the whole flow is reduced to  $\text{Re} \approx 5300$ . This should still be turbulent and is likely to be within the Reynolds number  
 331 independent regime. In fact, the convective boundary layer is very amenable to LES because the large coherent  
 332 structures with scales of order  $H$  dominate, and Sullivan and Patton (2011) show that ‘‘the majority of the low-order  
 333 moment statistics (means, variances, and fluxes) become grid independent when the ratio  $z_i/(Cs\Delta_f) > 310$ ’’. Here  $z_i$   
 334 is the inversion depth (i.e.  $H$ ),  $Cs$  is the Smagorinsky constant ( $\approx 0.2$ ), and  $\Delta_f$  essentially the grid length (so the actual  
 335 filter scale is a multiple of this). This implies  $\Delta_f < z_i/(310Cs) \approx 16 \text{ m}$  in this case. Hence our notional 1 m resolution  
 336 should be very well-converged LES.

337 Thus, provided the solution remains in the Re-independent turbulent regime, the relatively low Ra runs ( $\text{Ra} \geq 10^8$ )  
 338 may be interpreted as reasonable approximations to LES of much higher Ra (and hence Re) flows encountered in the  
 339 atmosphere. Indeed, a similar argument is made by Mellado et al. (2018) in a study of Stratocumulus convection,  
 340 except that they seem to have reversed the semantics of the conclusion by describing their artificially large viscosity  
 341 runs as DNS. This ‘‘DNS in a Re-independent regime’’ is, we would argue, more correctly described as a form of LES  
 342 as its basis is precisely the same.

343 A slight note of caution may arise from consideration of the boundary conditions, as the turbulence length scale  
 344 collapses as one approaches the boundary and buoyancy effects on turbulence become more dominant. (The same  
 345 concerns apply to LES). With a fixed heat-flux boundary condition, the concern is less as the surface exchange serves  
 346 merely to transport the given surface flux into the fluid where large eddies can start to transport it. In practice,  
 347 our results are similar for fixed temperature and fixed heat flux boundary conditions, suggesting that, so long as the  
 348 thermal boundary-layer is adequately resolved the solutions remain applicable to higher Re.

### 349 2.3 | Phenomenology of RBC

350 Direct numerical simulations of 2D, dry, Boussinesq Rayleigh-Bénard convection were performed for the range  $10^2 \leq$   
 351  $\text{Ra} \leq 10^{10}$  for a fluid with Prandtl number 0.707 (the value for dry air at standard temperature and pressure). For each  
 352 Ra, the fluid was initialized from the hydrostatically-balanced resting state (10), with small random perturbations to

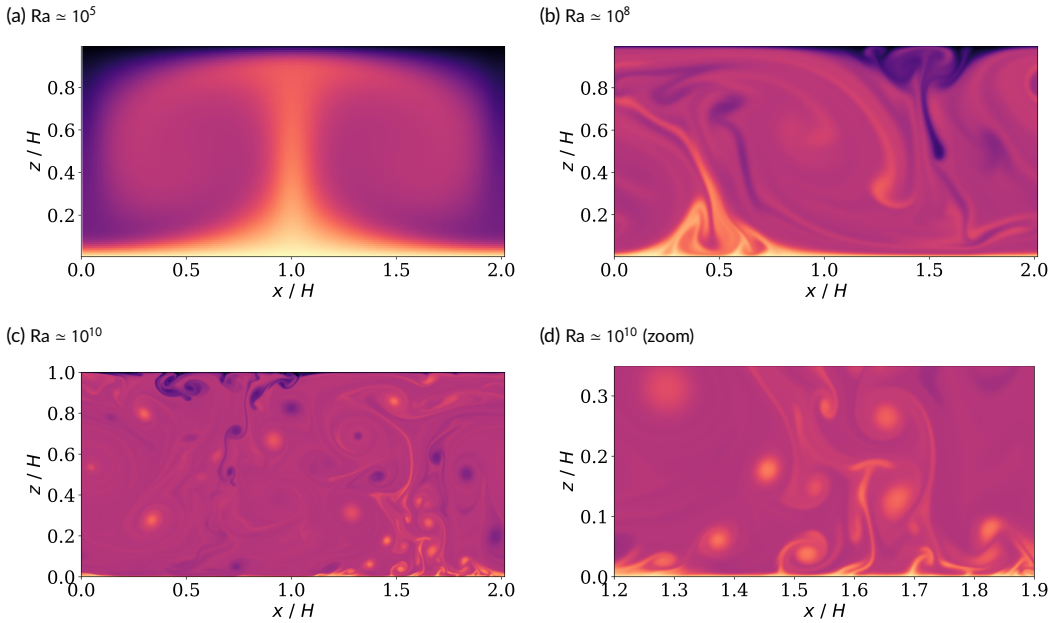


FIGURE 1 Snapshots of buoyancy fields in 2D Rayleigh-Bénard convection at varying Rayleigh number. In (a), the flow is convective but steady; in (b), the flow is turbulent, but only just, with  $Re \approx 5000$ ; in (c), the flow is highly turbulent and exhibits many small scale features; (d) is the same flow as (c) but zoomed in to show small-scale features close to the lower boundary layer, and also to demonstrate the resolution.

353 the buoyancy field  $|\delta b_{\text{pert}}| \leq 0.01\Delta B$  drawn from a uniform distribution. The aspect ratio of the domain was set equal  
 354 to the critical wavelength:  $\Gamma = L_x/L_z = \lambda_c/H \approx 2.02$  (for  $10^2 \leq Ra \leq 10^8$ , simulations were also run with  $\Gamma = 10$ , which  
 355 gave the same results for  $Nu$ ,  $Re$  etc.; therefore only the smaller aspect ratio results are reported). Each simulation  
 356 was run until a statistically-steady equilibrium was reached, determined by the convergence of the time-mean values  
 357 of  $Nu$ ,  $Re$ ,  $\delta_b$ , and the equivalence of the four methods of estimating  $Nu$ .

358 Since  $Nu \approx Nu_w \approx \varepsilon_b \approx 1 + \varepsilon_u/Ra$  for all simulations (not shown), verifying statistical steadiness, only  $Nu$  is  
 359 discussed hereafter. All three methods of estimating the Reynolds number also produce very similar results (fig. 2b),  
 360 and the free-convective scaling (with proportionality factor  $\approx 0.4$ ) gives good agreement with the observed scaling,  
 361 especially for  $Ra \gtrsim 10^6$ .

362 Figure 1 shows single-time snapshots of the 2D buoyancy field in fully developed RBC at various Rayleigh num-  
 363 bers. The solutions show several characteristic regimes. For  $Ra < Ra_c$ , diffusion damps out any motion and the  
 364 solution is entirely diffusive (not shown). As  $Ra$  increases above  $Ra_{\text{crit}}$  the solution exhibits first steady convection (a),  
 365 then transitional turbulence (b), and finally fully-developed convective turbulence (c-d). This broad phenomenology is  
 366 valid in both 2D and 3D, so for the remainder of the paper we restrict to 2D. Reproducing this phenomenology serves  
 367 both to demonstrate the usefulness of RBC as a model of convection, and to validate the chosen numerical method.

368 The scalings of  $Nu$ ,  $Re$ , and  $\delta_b$  are shown in Fig. 2, along with snapshots of buoyancy fields from representa-  
 369 tive simulations in each phenomenological regime in figure 1. A transition from diffusive to convective behaviour is  
 370 observed in both the Nusselt (figure 2a) and Reynolds (figure 2b) numbers at  $Ra \approx 1700$ , in agreement with the pre-  
 371 diction  $Ra_c = 1708$ . A transition to turbulence follows between  $10^7 \lesssim Ra \lesssim 10^8$ , as expected given that  $Re \approx 2000$

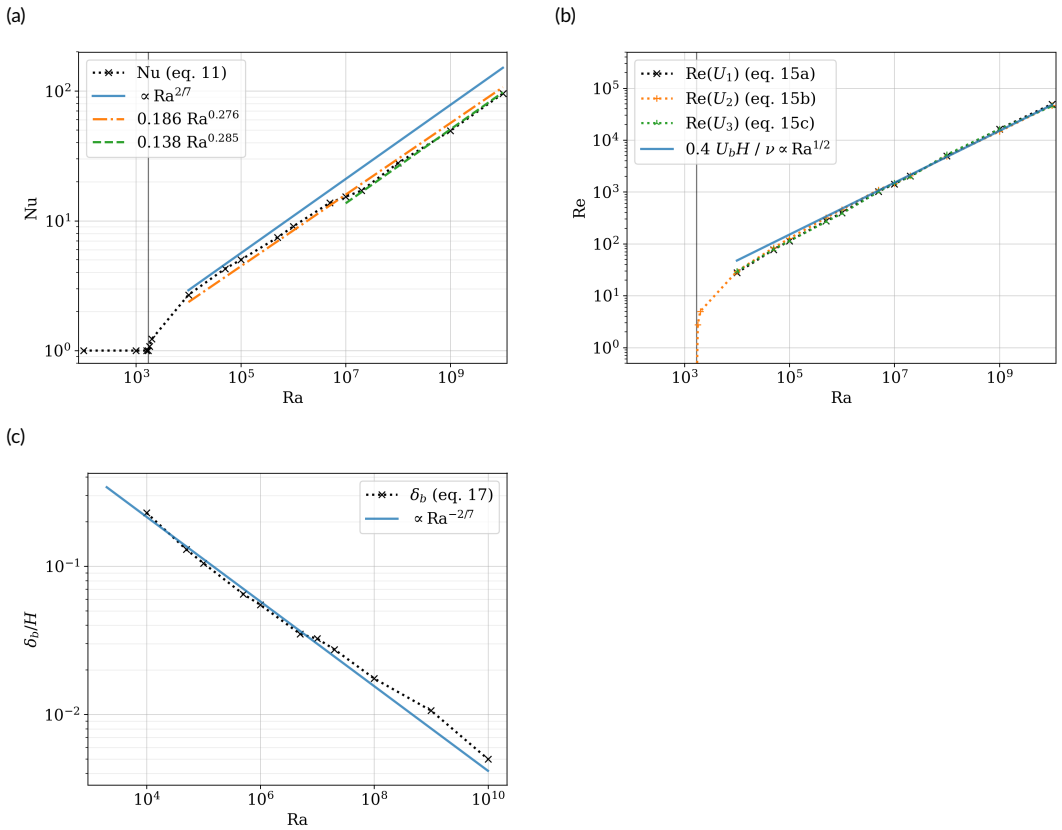


FIGURE 2 Validation of 2D Rayleigh-Bénard direct numerical simulations, showing scaling with applied buoyancy forcing,  $Ra$ , of: (a) heat transport ( $Nu$ ); (b) momentum transport ( $Re$ ); and (c) thermal boundary layer thickness ( $\delta_b$ ). In (a)-(c), the black crosses joined by a dotted line denote our main results. In (a) and (b), the solid black vertical line marks the theoretical critical Rayleigh number,  $Ra_c \approx 1708$ . In (a) the solid blue line follows the theoretical  $Nu \propto Ra^{2/7}$  scaling; the orange dash-dotted line follows the best fit line of Kerr (1996),  $Nu = 0.186 Ra^{0.276}$  (3D); the green dashed line follows the best fit of Johnston and Doering (2009),  $Nu = 0.138 Ra^{0.285}$  (2D), valid above  $Ra \approx 10^7$ . In (b) the three dotted lines show Reynolds numbers calculated from the alternative definitions in equation (15); the theoretical scaling,  $Re \propto Ra^{1/2}$ , is shown as a solid blue line. In (c), the solid blue line shows the theoretical scaling,  $\delta_b \propto Ra^{-2/7}$ .

372 for  $Ra \approx 2 \times 10^7$ . This can be seen in the qualitative nature of the flow: figure 1a is steady, representative of all flows  
 373 with  $Ra_c \lesssim Ra \lesssim 10^7$ ; while above  $Ra \gtrsim 2 \times 10^7$  the flow is intermittent and exhibits patterns on multiple scales,  
 374 characteristic of turbulence, as seen in Figs. 1b-d.

375 The Nusselt number obeys a power law close to  $Ra^{2/7}$ , and the Reynolds number a power law close to  $Ra^{1/2}$ , from  
 376 shortly after the onset of convection to the highest Rayleigh number considered. These are the expected exponents  
 377 within this parameter regime (Ahlers et al., 2009; Chillà and Schumacher, 2012). The three different possibilities for  
 378 the velocity scale in the Reynolds number calculation give similar results. A reduction in the prefactor of the power  
 379 law for  $Nu$  is observed between  $10^7 < Ra < 10^8$ , which coincides with the onset of turbulence. A similar transition

380 is seen in the results of Johnston and Doering (2009) for finite-difference DNS of 2D dry RBC with  $Pr = 1$ . Above  
 381  $Ra \approx 10^7$  they observe a power law relationship between  $Ra$  and  $Nu$  of  $Nu = 0.138 Ra^{0.285}$ , which our data are in  
 382 excellent agreement with.

383 Any two-fluid parametrization of RBC should therefore aim to capture the described scaling behaviour of  $Nu$  and  
 384  $Re$  with  $Ra$ .

### 385 3 | MULTI-FLUID EQUATION SET AND CLOSURE CHOICES

386 As a first step towards building a multi-fluid parametrization of convective turbulence, we motivate and present a  
 387 two-fluid single-column model of Rayleigh-Bénard convection. The full viscous multi-fluid Boussinesq equation set is  
 388 (Shipley et al., 2021):

$$389 \quad \frac{\partial \sigma_i}{\partial t} + \nabla \cdot (\sigma_i \mathbf{u}_i) = \overline{S_i^+} - \overline{S_i^-}, \quad (21)$$

$$390 \quad \begin{aligned} \frac{\partial \sigma_i \mathbf{u}_i}{\partial t} + \nabla \cdot (\sigma_i \mathbf{u}_i \otimes \mathbf{u}_i) &= \sigma_i b_i \hat{\mathbf{k}} - \sigma_i \nabla \overline{P} - \nabla (\sigma_i \rho_i) - \left[ \overline{P} \nabla \sigma_i - \overline{P \nabla I_i} \right] \\ &+ \nu \nabla^2 \sigma_i \mathbf{u}_i - \nu \nabla \cdot (\mathbf{u} \otimes \nabla I_i)^T - \nu \nabla I_i \cdot (\nabla \mathbf{u})^T \\ &+ \overline{\mathbf{u} S_i^+} - \overline{\mathbf{u} S_i^-} - \nabla \cdot (\overline{I_i \mathbf{u} \otimes \mathbf{u}} - \sigma_i \mathbf{u}_i \otimes \mathbf{u}_i), \end{aligned} \quad (22)$$

$$391 \quad \begin{aligned} \frac{\partial \sigma_i b_i}{\partial t} + \nabla \cdot (\sigma_i \mathbf{u}_i b_i) &= \kappa \nabla^2 \sigma_i b_i - \kappa \nabla I_i \cdot \nabla \overline{b} - \kappa \nabla \cdot \overline{b \nabla I_i} \\ &+ \overline{b S_i^+} - \overline{b S_i^-} - \nabla \cdot (\overline{I_i \mathbf{u} b} - \sigma_i \mathbf{u}_i b_i), \end{aligned} \quad (23)$$

$$392 \quad \sum_i \nabla \cdot (\sigma_i \mathbf{u}_i) = 0. \quad (24)$$

$$393 \quad \sum_i \sigma_i = 1. \quad (25)$$

395 Here an overbar denotes a spatial filter (Germano, 1992);  $i \in \{0, 1, \dots, n\}$  indexes the fluid partitions;  $I_i$  is an indicator  
 396 function for fluid  $i$ ;  $\sigma_i := \overline{I_i}$  is the fraction of fluid  $i$  contained within a characteristic filter volume;  $\mathbf{u}_i := \overline{I_i \mathbf{u}} / \sigma_i$   
 397 and  $b_i := \overline{I_i b} / \sigma_i$  are the velocity and buoyancy fields of fluid  $i$ ;  $\rho_i := \overline{I_i P} / \sigma_i - \overline{P}$  is the difference between the  
 398 conditionally-filtered pressure in fluid  $i$  and the unconditionally filtered pressure  $\overline{P}$ ;  $\overline{S_i^\pm}$ ,  $\overline{\mathbf{u} S_i^\pm}$ ,  $\overline{b S_i^\pm}$  are respectively  
 399 sources and sinks of fluid fraction, momentum, and buoyancy in fluid  $i$  arising from the relabelling of fluid. The  
 400 unconditionally-filtered pressure,  $\overline{P}$ , ensures the incompressibility of the mean flow, equation (24).

401 Equations (21)-(25) are derived by conditionally spatially filtering the Boussinesq equations (1)-(3) in the manner  
 402 set out by Thuburn et al. (2018); however, here viscous terms and sources and sinks of fluid fraction are retained from  
 403 the outset. The only terms neglected here are those arising from possible non-commutation of the spatial filter with  
 404 the partial derivatives. For a full derivation and discussion of the terms requiring closure, see Shipley et al. (2021).

#### 405 3.1 | Closures

406 The terms in equations (21)-(23) which require closure can be split into:

- 407 •  $\rho_i$ , the difference between the conditionally-filtered pressure in fluid  $i$  and the unconditionally filtered pressure;
- 408 •  $\overline{P} \nabla \sigma_i - \overline{P \nabla I_i}$ ,  $-\nu \nabla \cdot (\mathbf{u} \otimes \nabla I_i)^T - \nu \nabla I_i \cdot (\nabla \mathbf{u})^T$ , and  $-\kappa \nabla I_i \cdot \nabla \overline{b} - \kappa \nabla \cdot \overline{b \nabla I_i}$ , which arise from conditionally-filtering

- 409 the pressure gradient, viscous diffusion, and buoyancy diffusion terms;
- 410 •  $-\nabla \cdot (\overline{I_i \mathbf{u} \otimes \mathbf{u}} - \sigma_i \mathbf{u}_i \otimes \mathbf{u}_i)$ , and  $-\nabla \cdot (\overline{I_i \mathbf{u} b} - \sigma_i \mathbf{u}_i b_i)$ , which are often termed “subfilter fluxes” and are akin to the
- 411 Reynolds stress and subfilter buoyancy flux, respectively, in normal higher-order modelling of turbulence;
- 412 •  $\overline{S_i^\pm}, \overline{\mathbf{u} S_i^\pm}, \overline{b S_i^\pm}$ , which arise from filtering the re-labelling of fluid parcels.

413 We present closures that attempt to model the dominant coherent overturning structures of RBC (seen in the DNS,

414 figure 1).

415 For this study, differences between conditionally-filtered and unconditionally-filtered pressures are parametrized

416 as  $p_i = (\sum_j \sigma_j \gamma_i \nabla \cdot \mathbf{u}_j) - \gamma_i \nabla \cdot \mathbf{u}_i$ , where  $\gamma_i$  is a volume (or “bulk”) viscosity. This has successfully been used by Weller

417 et al. (2020), where it was argued that such a form is plausible since in the underlying Boussinesq flow, the pressure is

418 simply a Lagrange multiplier to enforce the divergence-free condition. It is also possible to derive this form by analogy

419 with the “bulk viscous pressure” which arises in compressible fluid dynamics, as in Batchelor (1967) – see Shipley et al.

420 (2021) for details.

421 Residual terms arising from conditionally-filtering the pressure gradient and diffusion terms are closed via a mean-

422 field approximation:

- 423 •  $\overline{P \nabla \sigma_i} - \overline{P \nabla I_i} \rightarrow \overline{P} \nabla \sigma_i - \overline{P} \nabla \sigma_i = 0;$
- 424 •  $-\nu \nabla \cdot (\overline{\mathbf{u} \otimes \nabla I_i})^\top - \nu \nabla I_i \cdot (\nabla \mathbf{u})^\top \rightarrow -\nu \nabla \cdot (\overline{\mathbf{u}} \otimes \nabla \sigma_i)^\top - \nu \nabla \sigma_i \cdot (\nabla \overline{\mathbf{u}})^\top;$
- 425 •  $-\kappa \nabla I_i \cdot \nabla \overline{b} - \kappa \nabla \cdot \overline{b \nabla I_i} \rightarrow -\kappa \nabla \sigma_i \cdot \nabla \overline{b} - \kappa \nabla \cdot \overline{b \nabla \sigma_i}.$

426 These choices retain the correct sum over all fluids for the entire pressure, viscous, and diffusive terms, respectively.

427 They also cause the fluid fractions to behave passively in the case of two fluids, and in the absence of transfers: the

428 Eulerian derivatives for  $\mathbf{u}_i$  and  $b_i$  do not depend on  $\sigma_i$  if the two fluids have the same  $\mathbf{u}_i$  and  $b_i$ .

429 The resolved velocities and buoyancies of the multi-fluid split are assumed to dominate the single-fluid subfilter

430 fluxes, such that  $\overline{I_i \mathbf{u} \otimes \mathbf{u}} \approx \sigma_i \mathbf{u}_i \otimes \mathbf{u}_i$  and  $\overline{I_i \mathbf{u} b} \approx \sigma_i b_i \mathbf{u}_i$ . This is the same as assuming that the multi-fluid split captures

431 all of the subfilter variability in the momentum and buoyancy fluxes, i.e. neglecting the residual subfilter fluxes of

432 momentum and buoyancy,  $\nabla \cdot (\overline{I_i \mathbf{u} \otimes \mathbf{u}} - \sigma_i \mathbf{u}_i \otimes \mathbf{u}_i)$  and  $\nabla \cdot (\overline{I_i \mathbf{u} b} - \sigma_i \mathbf{u}_i b_i)$ . While this will never be exactly true, it is

433 instructive to see how well a multi-fluid model with no extra subfilter modelling can perform when simulating a fully

434 turbulent flow. In the single column context this requires the vertical grid to adequately resolve the boundary layers,

435 as in the DNS.

436 To proceed further, we must decide what the labels  $I_i$  represent. The simplest choice is to restrict to two fluids;

437 the symmetries of the Rayleigh-Bénard problem suggest choosing one falling and the other rising: let  $i = 0$  denote

438 fluid with  $w \leq 0$ , and  $i = 1$  denote fluid with  $w > 0$  (as in Weller et al., 2020). Then fluid 1 represents “updrafts” while

439 fluid 0 represents “downdrafts”. This choice of definitions for the two fluids, coupled with the discrete symmetry of

440 the unfiltered equations under the simultaneous transformations  $z \rightarrow \frac{H}{2} - z$ ,  $b \rightarrow -b$ , forces  $\int_D \sigma_i dV = \frac{1}{2}$ . This

441 constraint can be used as a “sanity check” for both the initial conditions and the transfer terms  $\mathcal{S}_i^\pm$ . The discrete

442 symmetry of the fluids under exchange also forces  $\gamma_i = \gamma_j$  if  $\gamma$  is not a function of  $z$ .

443 Specializing to two fluids allows the sources of fluid fraction  $i$  to be written as  $\overline{S_i^\pm} = \sigma_j S_{ji}$ , where  $\sigma_j S_{ji}$  is the rate

444 of transfer of fluid fraction from  $j$  to  $i$ . A similar relation follows for the sinks. We choose to model the exchanges

445 of momentum and buoyancy from fluid  $i$  to  $j$  as a characteristic value,  $\mathbf{u}_{ij}^T$  or  $b_{ij}^T$ , times the rate of transfer of fluid

446 fraction from  $i$  to  $j$ ,  $\sigma_i S_{ij}$ . This aligns with the modelling approach taken in other recent works on multi-fluid modelling

447 (Thuburn et al., 2018, 2019; Weller and McIntyre, 2019; Weller et al., 2020; McIntyre et al., 2020).

448 Partitioning the flow based on the sign of  $w$  forces  $w_{ij}^T = 0$ . For a single-column model, it remains only to specify



449 the form of the fluid fraction transfer rate,  $S_{ij}$ , and the transferred buoyancy,  $b_{ij}^T$  (for a 2D or 3D model, the horizontal  
450 components of the transferred velocity would also need to be specified). For the fluid fraction transfer rate we choose

$$451 \quad S_{ij} = \max(-\nabla \cdot \mathbf{u}_i, 0), \quad (26)$$

453 which in 1D is similar to dynamical entrainment, and follows the successful implementation of the same divergence-  
454 based transfer in Weller et al. (2020). This aims to capture the large-scale overturning circulation, and is exactly  
455 correct for the first normal mode of RBC with stress-free boundaries (Shipley et al., 2021). McIntyre (2020, chapter 2)  
456 also shows that this choice of transfer rate removes the problematic Kelvin-Helmholtz-like instability for a two-fluid  
457 Boussinesq system (Thuburn et al., 2019).

458 The transferred buoyancy must depend on the distribution of buoyancy within each fluid, and on the detailed  
459 dynamics of the relabelling. In the absence of this information, we choose a simple model:

$$460 \quad b_{ij}^T = b_i + (-1)^i C |b_i|, \quad (27)$$

462 with some dimensionless constant  $C \geq 0$ . That is, the buoyancy of fluid parcels relabelled from  $i$  to  $j$  is modelled as  
463 the mean buoyancy within the fluid  $i$  plus or minus some constant times the magnitude of the buoyancy, to crudely  
464 approximate the subfilter buoyancy variability. The signs are chosen to model the fact that the fluid transferred from  
465 the falling (0) to the rising (1) fluid is expected to be more buoyant than the average falling fluid parcel for that height,  
466 while the reverse should be true for transfers from the rising (1) to the falling (0) fluid. This is a similar formulation to  
467 that used by Thuburn et al. (2019), though in theirs the transferred value depends on both the initial and destination  
468 fluids, rather than just the initial fluid.

469 Making these closure assumptions reduces the equation set to:

$$470 \quad \frac{\partial \sigma_i}{\partial t} + \nabla \cdot (\sigma_i \mathbf{u}_i) = \sigma_j S_{ji} - \sigma_i S_{ij}, \quad (28)$$

$$471 \quad \begin{aligned} \frac{\partial \sigma_i \mathbf{u}_i}{\partial t} + \nabla \cdot (\sigma_i \mathbf{u}_i \otimes \mathbf{u}_i) &= \sigma_i b_i \hat{\mathbf{k}} - \sigma_i \nabla \bar{P} - \nabla (\sigma_i p_i) \\ &+ \nu \nabla^2 \sigma_i \mathbf{u}_i - \nu \nabla \cdot (\bar{\mathbf{u}} \otimes \nabla \sigma_i)^\top - \nu \nabla \sigma_i \cdot (\nabla \bar{\mathbf{u}})^\top \\ &+ \sigma_j \mathbf{u}_{ji}^T S_{ji} - \sigma_i \mathbf{u}_{ij}^T S_{ij}, \end{aligned} \quad (29)$$

$$472 \quad \begin{aligned} \frac{\partial \sigma_i b_i}{\partial t} + \nabla \cdot (\sigma_i \mathbf{u}_i b_i) &= \kappa \nabla^2 \sigma_i b_i - \kappa \nabla \sigma_i \cdot \nabla \bar{b} - \kappa \nabla \cdot \bar{b} \nabla \sigma_i \\ &+ \sigma_j b_{ji}^T S_{ji} - \sigma_i b_{ij}^T S_{ij}, \end{aligned} \quad (30)$$

474 with  $i \in \{0, 1\}$ , and the specific parametrization choices:

$$475 \quad S_{ij} = \max(-\nabla \cdot \mathbf{u}_i, 0), \quad (31)$$

$$476 \quad \mathbf{w}_{ij}^T = 0, \quad (32)$$

$$477 \quad b_{ij}^T = b_i + (-1)^i C |b_i| \quad (33)$$

$$478 \quad p_i = \left( \sum_j \sigma_j \gamma \nabla \cdot \mathbf{u}_j \right) - \gamma \nabla \cdot \mathbf{u}_i. \quad (34)$$

479

480 The equations are given in vector form because of the desire to eventually create a 3D grey-zone convection parametriza-

481 tion; to that end the subsequent numerical method is also three-dimensional. Note, however, that in the form (28)-(34),  
 482 the horizontal components of the transferred velocity still require closure.

### 483 3.1.1 | Boundary conditions

484 Conditionally filtering the boundary conditions for RBC gives  $\mathbf{u}_i(z=0, H) = \mathbf{0}$ ,  $b_i(z=0, H) = \pm \Delta B/2$ . The Neumann  
 485 boundary condition for the unconditionally filtered pressure (required for the numerical solution, which solves elliptic  
 486 equations for the pressures) is hydrostatic,  $\frac{d\bar{p}}{dz}(z=0, H) = \bar{b}(z=0, H)$ . Boundary conditions on the perturbation  
 487 pressures are chosen to be zero-gradient,  $\frac{d p_i}{dz}(z=0, H) = 0$ .

488 Because the  $\sigma_i$  equation is a transport equation with no diffusion, boundary values of  $\sigma_i$  are not in the domain of  
 489 dependence of its solution. The asymptotic boundary behaviour of  $\sigma_i$  is thus entirely dependent on the asymptotic  
 490 behaviour of the transfer terms as the boundaries are approached. Boundary values of  $\sigma_i$  are however required for  
 491 the momentum and buoyancy equations, which do contain second derivatives of  $\sigma_i$ . These boundary values should  
 492 be set by extrapolated values of  $\sigma_i$  from the interior of the domain. However, for this study we choose zero-gradient  
 493 conditions for  $\sigma_i$  for better numerical behaviour. Heuristically this means that we are imposing no creation of fluid in  
 494 either partition at the boundary.

### 495 3.2 | Scaling of pressure differences between fluids

496 In single-column form, equations (28)-(34) contain two free parameters:  $\gamma$  and  $C$ .  $C$  is dimensionless and should be  
 497  $\lesssim O(1)$ , but  $\gamma$  has the dimensions of (bulk) viscosity and does not have an obvious magnitude. In this section we  
 498 present a scaling argument for  $\gamma$  with the external dimensionless control parameters  $Ra, Pr$ , thus reducing the model  
 499 to the choice of two dimensionless constants which should both be  $O(1)$ .

500 In convection, a distinction is often made between filamentary plumes and a well-mixed environment; this dis-  
 501 tinction is clearly seen in the example RBC buoyancy fields of figure 1, and is the basis of the conceptual "updraft"-  
 502 "environment" partition. We assume that such a plume has a length  $O(H)$ , a width  $\delta$ , and the along-plume flow scales  
 503 with the large-scale circulation  $U \sim U_B = \sqrt{\Delta B H}$ . Orienting a local Cartesian co-ordinate system such that  $\hat{\mathbf{x}}$  points  
 504 parallel to the plume and  $\hat{\mathbf{z}}$  points normal to it, the scaled continuity equation gives:

$$505 \quad \frac{U}{H} \frac{\partial \bar{u}}{\partial \bar{x}} = -\frac{W}{\delta} \frac{\partial \bar{w}}{\partial \bar{z}} \quad \implies \quad W = U \frac{\delta}{H}. \quad (35)$$

507 Splitting the buoyancy equation similarly into its plume-parallel and -normal parts gives:

$$508 \quad \left( \frac{\partial \bar{b}}{\partial \bar{t}} + \frac{\partial \bar{u} \bar{b}}{\partial \bar{x}} + \frac{\partial \bar{w} \bar{b}}{\partial \bar{z}} \right) = \frac{\kappa T_b}{\delta^2} \left( \frac{\delta^2}{H^2} \frac{\partial^2 \bar{b}}{\partial \bar{x}^2} + \frac{\partial^2 \bar{b}}{\partial \bar{z}^2} \right). \quad (36)$$

510 Note the buoyancy scaling cancels here. The simplest choice of the time scale is  $T_b = \delta^2 / \kappa$ , which makes the coeffi-  
 511 cient of the final term on the RHS one, consistent with filamentary plumes being diffusion-limited in well-developed  
 512 turbulent flows. Scaling the plume-parallel momentum equation with time scale  $T_m = T_b / Pr$ , buoyancy with  $\Delta B$  and  
 513 pressure with  $P \sim U^2$  (Bernoulli scaling), leads to:

$$514 \quad \frac{\partial \bar{u}}{\partial \bar{t}} + \frac{\partial \bar{u} \bar{u}}{\partial \bar{x}} + \frac{\partial \bar{u} \bar{w}}{\partial \bar{z}} = Re \frac{\delta^2}{H^2} \left( -\frac{\partial \bar{p}}{\partial \bar{x}} + \bar{b} \hat{\mathbf{g}} \cdot \hat{\mathbf{x}} \right) + \left( \frac{\delta^2}{H^2} \frac{\partial^2 \bar{u}}{\partial \bar{x}^2} + \frac{\partial^2 \bar{u}}{\partial \bar{z}^2} \right), \quad (37)$$

516 where  $\text{Re} = UH/\nu = \text{Pr}^{-1/2} \text{Ra}^{1/2}$ . The pressure gradient and buoyancy terms are assumed to drive the flow, and so  
 517  $\text{Re} \delta^2/H^2 = O(1)$  and:

$$518 \quad \frac{\delta}{H} = \text{Re}^{-1/2}. \quad (38)$$

520 Hence the across-plume pressure contrast – i.e. the difference in pressure between the plume and the bulk – may  
 521 be scaled as  $P_z = P\delta/H = \Delta B\delta$ .

522 These results are the standard Prandtl-Blasius results with  $\delta$  the boundary-layer depth, consistent with the pre-  
 523 sumption that plumes in RBC are simply detached from the boundary layers. This is a standard assumption for the  
 524 kinetic boundary layer depth in scaling analysis of RBC, for example in the successful theory of Grossmann and Lohse  
 525 (2000) for the Nusselt and Reynolds number scalings. The  $\text{Re} \propto \text{Ra}^{1/2}$  result is also expected for RBC in the parameter  
 526 regimes under study in this paper (Ahlers et al., 2009, table 2).

527 We wish to parametrize the difference between the conditionally-filtered pressure in partition  $i$ , and the unconditionally-  
 528 filtered pressure, as a bulk viscous stress:  $p_i = -\gamma(\nabla \cdot \mathbf{u}_i - \sum_j \sigma_j \nabla \cdot \mathbf{u}_j)$ , equation (34). Assuming that the multi-fluid  
 529 split is dominated by a plume vs. bulk contrast, then  $\mathbf{u}_i$  scales with the velocity of the plumes,  $\sqrt{\Delta B H}$ , and the diver-  
 530 gence within each fluid should then scale as  $\nabla \cdot \mathbf{u}_i = (U/H)\tilde{\nabla} \cdot \tilde{\mathbf{u}}_i$  (so long as the filter width is  $\gtrsim O(H)$ ). Collecting  
 531 the nondimensionalized expressions for the pressure and the bulk viscous stress gives:

$$532 \quad \gamma \frac{U}{H} \tilde{\nabla} \cdot \tilde{\mathbf{u}}_i = \Delta B \delta \frac{\partial \tilde{p}}{\partial \tilde{z}}$$

$$533 \quad \implies \frac{\gamma}{\nu} = O(1) \times \frac{\Delta B H}{\nu U} \delta = O(1) \times \frac{U^2 H}{\nu U} \frac{\delta}{H} = O(1) \times \text{Re}^{\frac{1}{2}}$$

$$534 \quad \implies \frac{\gamma}{\nu} = \hat{\gamma}_0 \text{Ra}^{1/4} \text{Pr}^{-1/4}, \quad (39)$$

536 introducing the  $O(1)$ , dimensionless constant  $\hat{\gamma}_0$ .

537 This scaling law for  $\gamma(\text{Ra}, \text{Pr})$  reduces the model for the pressure perturbation to the specification of an  $O(1)$   
 538 constant,  $\hat{\gamma}_0$ . Although  $\hat{\gamma}_0$  must be determined empirically, this determination need only be performed at one Rayleigh  
 539 number. Since  $\text{Pr} = 0.707$  is constant throughout our experiments, we choose to subsume the factor of  $\text{Pr}^{-1/2} \approx 1.19$   
 540 into the definition of  $\hat{\gamma}_0$  from now on.

## 541 | 4 | NUMERICAL METHODS

### 542 | 4.1 | Single-fluid solver

543 Single-fluid reference solutions (section 2.1) were computed using the single-fluid Boussinesq finite volume code  
 544 `boussinesqFoam` (available at [www.github.com/AtmosFOAM/AtmosFOAM](http://www.github.com/AtmosFOAM/AtmosFOAM)). This solves the single-fluid Boussinesq  
 545 equation set (5)-(6) using precisely the same numerical method as detailed below for the multi-fluid equation set, but  
 546 with only one fluid. This single-fluid solver gives statistically identical results to the multi-fluid solver when the latter  
 547 is run with no coupling terms between the fluids, such that the  $\sigma_i$  are simply passive tracers.

### 548 | 4.2 | Two-fluid solver

549 The two-fluid Boussinesq equation set (30)-(34) is solved in advective form using the finite volume solver `multiFluidBoussinesqFoam`  
 550 this is part of the `AtmosFOAM` library of CFD codes for atmospheric fluid dynamics, based on the `OpenFOAM` open-source

551 CFD library. The code is available at [www.github.com/AtmosFOAM/AtmosFOAM-multiFluid](https://www.github.com/AtmosFOAM/AtmosFOAM-multiFluid). The method is similar  
 552 to that detailed in section 3 of Weller et al. (2020); an overview, and choices specific to this paper, are presented  
 553 below.

554 The spatial discretization uses Arakawa C-grid staggering in the horizontal and Lorenz staggering in the vertical.  
 555 Temporal discretization is Crank-Nicolson with off-centring coefficient  $\alpha = 0.55$ .

556 Prognostic variables are  $b_i$  and  $\sigma_i$  at cell centres, and the volume flux  $\phi_i := \mathbf{u}_i \cdot \mathbf{S}_f$  at cell faces, where  $\mathbf{S}_f$  is the  
 557 outward-pointing area vector of face  $f$ . Advection of  $b_i$  and  $\sigma_i$  is total variation-diminishing (with a van Leer limiter) to  
 558 preserve boundedness, while advection of  $\phi_i$  is linear upwind. Thus the spatial discretization is (almost) second-order  
 559 accurate.

560 The transfer terms  $S_{ij}$  are handled explicitly, while the momentum and buoyancy transfers are implicit and operator-  
 561 split, as in (Weller and McIntyre, 2019; McIntyre et al., 2020; Weller et al., 2020).

562 Diagnostic variables are the pressures  $P$  and  $p_i$  at cell centres. Solutions for both  $P$  and  $p_i$  are implicit but not  
 563 simultaneous: first a Poisson equation is solved for  $P$ , which maintains a divergence-free mean velocity field (i.e. it  
 564 ensures eq. (24) is satisfied), followed by a Helmholtz equation for each  $p_i$ . These solutions are then iterated to  
 565 convergence. The generalized Geometric-Algebraic MultiGrid (GAMG) method is used for the implicit pressure solves,  
 566 with an absolute tolerance of  $10^{-6}$ .

567 Two outer iterations (for the whole of the above method) and two inner iterations (for the implicit pressure solves)  
 568 are performed per time-step.

569 Apart from the transfer terms, this method is suitable for an arbitrary number of fluids, in up to 3 spatial dimen-  
 570 sions. However, the transfer terms, and their inclusion into the algorithm, are currently specific to two fluids.

## 571 5 | TWO-FLUID SINGLE-COLUMN MODEL RESULTS

572 For  $10^2 \leq \text{Ra} \leq 10^{10}$ , single-column two-fluid simulations were run with the same vertical resolution as the reference  
 573 DNS (see table 1) for various values of  $\hat{\gamma}_0$  and  $C$ . The qualitative nature of the solutions is described in section 5.1,  
 574 followed by an analysis of sensitivity to the choice of  $\hat{\gamma}_0$  and  $C$  in section 5.2. In section 5.3 the global buoyancy and  
 575 momentum transport,  $\text{Nu}$  and  $\text{Re}$ , is examined as a function of the buoyancy forcing  $\text{Ra}$ .

576 For all simulations, the initial state was constructed from a resting hydrostatically-balanced solution with a linear  
 577 buoyancy profile and uniform  $\sigma_i = 0.5$  in both fluids. Small non-zero velocities equal to  $\pm 10^{-3} U_B$  were added to  
 578 ensure correct labeling, and random perturbations of magnitude  $|\delta b| \leq 0.0008 \Delta B$  drawn from a uniform distribution  
 579 were added to the initial linear profile to seed instability<sup>5</sup>. Simulations were run until a steady state was reached  
 580 ( $9-12T_e$ ); the steady-state profiles of buoyancy, pressure, vertical velocity, and fluid fraction, were then compared with  
 581 the corresponding statistically steady-state time-mean conditionally horizontally averaged DNS profiles. Resolutions,  
 582 time-step size, and total simulation run time for each simulation are given in table 2.

583 The single column model spins up to equilibrium in a remarkably similar manner to the horizontally-averaged  
 584 DNS; this is demonstrated in figure 3, which shows the Nusselt number vs. time for both DNS and single-column  
 585 simulations at  $\text{Ra} = 10^5$  and  $10^8$ . For these simulations,  $\hat{\gamma}_0 = 1.861$ , and  $C = 0.5, 0$  for  $\text{Ra} = 10^5, 10^8$ , respectively  
 586 (see section 5.3). At each  $\text{Ra}$ , convection initiates at a similar time ( $\approx 2T_e$ ) in both the single-column and DNS flows,  
 587 seen in the sharp increase in  $\text{Nu}$  above the purely diffusive value of 1. This initial convective surge causes a strong  
 588 peak in the Nusselt number (slightly overestimated by the single-column model), before the system gradually settles

<sup>5</sup>This value was chosen in order to approximate the same initial available potential energy in both the DNS and the single-column simulations. However, the (linear) growth rate of instabilities in a single fluid is not dependent on the size of the initial perturbation, and so the exact magnitude of the initial perturbations does not matter so long as it is small.

Ra	$T_{\text{tot}}/4T_B$	$\Delta t/4T_B$
$10^2$	19	$1.998 \times 10^{-4}$
$10^3$	63	$3.197 \times 10^{-4}$
$2 \times 10^3$	38	$2.557 \times 10^{-4}$
$10^4$	19	$1.279 \times 10^{-3}$
$10^5$	19	$1.279 \times 10^{-3}$
$10^6$	19	$7.992 \times 10^{-4}$
$10^7$	19	$3.197 \times 10^{-4}$
$2 \times 10^7$	19	$5.115 \times 10^{-4}$
$10^8$	19	$3.197 \times 10^{-4}$
$10^9$	19	$1.598 \times 10^{-4}$
$10^{10}$	19	$5.115 \times 10^{-5}$

TABLE 2 Details of time-step size and total simulation time for the two-fluid single-column results (section 5). Resolutions are the same as the vertical resolution of the DNS, explained in section 2.1.1 and given in table 1. All two-fluid single-column simulations at a given Ra required similar time-steps regardless of  $\hat{\gamma}_0$  and  $C$ , therefore only the values for  $\hat{\gamma}_0 = 1.861$ ,  $C = 0.5$  ( $\text{Ra} \leq 10^7$ ),  $\hat{\gamma}_0 = 1.861$ ,  $C = 0$  ( $\text{Ra} > 10^7$ ) are given.

589 down towards equilibrium with decaying Nusselt number under- and overshoots. The under- and overshoots appear  
590 stochastic for the DNS, whereas they are periodic for the single-column model; that the single-column model appears  
591 less chaotic than the DNS is unsurprising.

592 The same steady state was reached when initializing from other initial conditions (e.g. initializing from the DNS  
593 reference profiles), provided the identities of the fluids were initialized correctly and the initial column-integrated  
594 fraction of fluid in each fluid was equal to 0.5. This suggests that the steady state is robust. Similar qualitative spin-up  
595 behaviour is also observed with different values of  $\hat{\gamma}_0$  and  $C$ . Thus, for the remainder of the paper we consider only  
596 the steady state, and not the spin-up.

597 We begin our study of the two-fluid single-column model steady-state by looking at the qualitative behaviour  
598 of the equilibrium profiles in different Rayleigh number regimes. We then investigate the sensitivity of those profiles  
599 to the two closure constants,  $C$  and  $\hat{\gamma}_0$ . Finally we examine the scaling of the global parameters Nu and Re with Ra  
600 produced by the model.

## 601 5.1 | Phenomenology

602 For each of the characteristic Rayleigh numbers  $\text{Ra} = 10^5, 10^8, 10^{10}$  (as in figure 1), we present and discuss an example  
603 two-fluid single column simulation. Rather than use the fixed value used above for discussion of the spin-up, the values  
604 of  $\hat{\gamma}_0$  and  $C$  in the example simulations were chosen to have the best qualitative fit to the conditionally horizontally  
605 averaged DNS for all profiles. The discussion for each of these examples qualitatively applies to all simulations within  
606 the characteristic Rayleigh number regime.

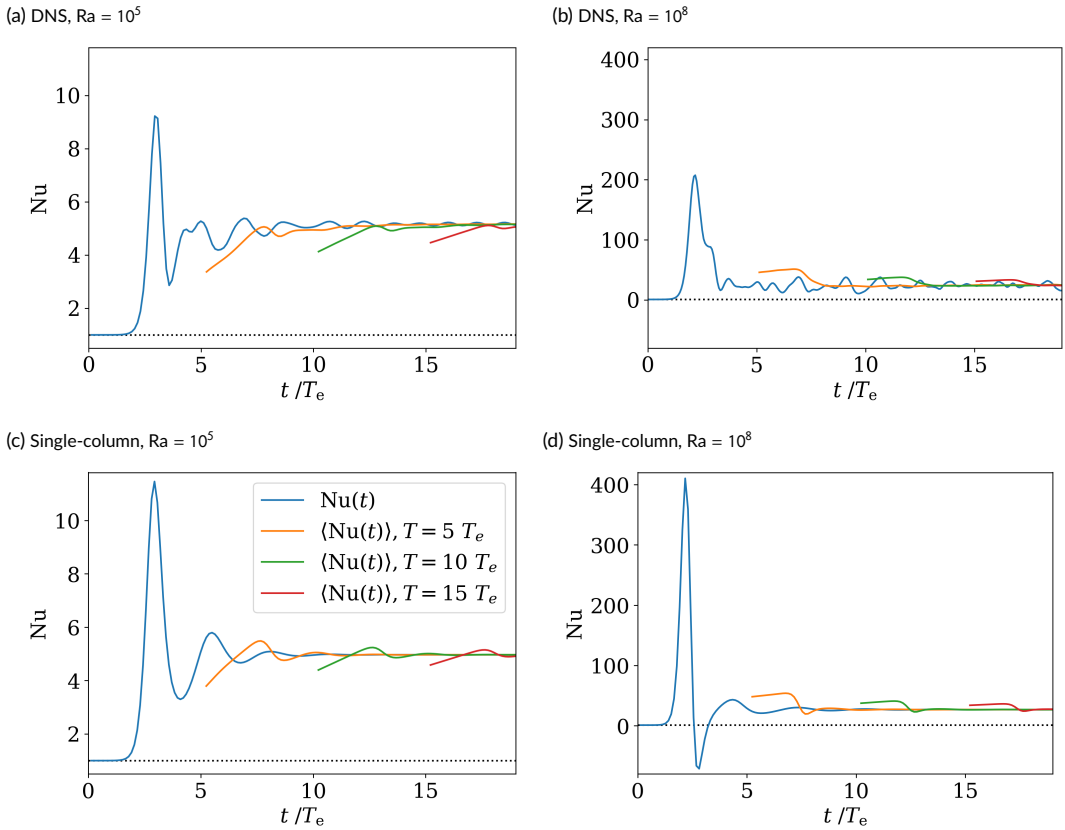


FIGURE 3 Nondimensionalized vertical heat flux vs. time for (a,b) DNS and (c,d) single-column models. In each subfigure, the blue curve shows the instantaneous nondimensionalized vertical buoyancy flux,  $H \times (wb - \kappa \frac{\partial b}{\partial z}) / \kappa \Delta B$ , while the orange, green, and red curves show Nusselt numbers (domain- and time-averaged nondimensionalized buoyancy flux) for different averaging times. In each plot,  $Nu = 1$  is shown as a black dotted line. In (c) and (d)  $\gamma/\nu = 1.861 \times Ra^{1/4}$ , with  $C = 0.5$  for (c) and  $C = 0$  for (d) (see figure 10a).

## 607 | Laminar ( $Ra = 10^5$ )

608 At  $Ra = 10^5$ , the DNS exhibits laminar convective rolls (see Fig. 1a). This solution is qualitatively characteristic of  
 609 the flow for all laminar  $Ra$ ,  $Ra_c < Ra \lesssim 10^7$ . Steady state results of a two-fluid single-column model governed by  
 610 equations (28)-(34) with  $\hat{\gamma}_0 \approx 0.75$ ,  $C = 0.5$  are shown in Fig. 4. The mean buoyancy (a) and pressure (b) profiles  
 611 match closely between the DNS and the single column model; in particular the model correctly predicts a well-mixed  
 612 buoyancy in the fluid interior, with a sharp buoyancy gradient close to the top and bottom boundaries. The shape of  
 613 the pressure profile is also correct, though the maxima are slightly too high close to the boundaries.

614 Good agreement is also seen between the DNS and two-fluid single column model for the individual fluid buoyancy  
 615 profiles: the overall shape is correct, though the profiles are too far apart in the middle of the domain, leading  
 616 to surplus buoyancy transport for a given velocity profile. Experiments varying  $C$  (see section 5.2.2) demonstrated  
 617  $C > 0$  was required to reproduce a buoyancy overshoot at the top (bottom) of the rising (falling) fluid. By overshoot,

618 we mean the part of the buoyancy profile at the interface between the bulk and the buoyancy boundary layer where  
 619  $\frac{db_i}{dz}$  changes sign. These overshoots can be seen in the 2D buoyancy field of the DNS flow of figure 1a and are a  
 620 general feature of  $O(1)$  Prandtl number laminar RBC. (For  $Pr > 1$ , the overshoots become so strong that they begin  
 621 to be seen even in the mean buoyancy profile; such profiles can be seen in e.g. Fig. 4b of Schmalzl et al. (2004).) The  
 622 value  $C = 0.6$  gives the best shape for  $b_i(z)$  for  $Ra = 10^5$ , but  $C \approx 0.5$  works for all laminar  $Ra$ .

623 The individual fluid velocity profiles are roughly the correct shape; the slight asymmetry in the location of the  
 624 maxima in each fluid in the DNS is due to the gradient of the volume fraction profile in the DNS (i.e. forcing the  
 625 correct gradient of  $\sigma_i$  reproduces the asymmetry in the vertical velocity profiles).

626 The pressure profiles with each fluid are captured by the scheme, suggesting that to leading order  $p_i \propto -\gamma \nabla \cdot \mathbf{u}_i$   
 627 is an appropriate model of the pressure differences. The model is particularly good close to the boundaries, but the  
 628 fluids are better mixed in the interior of the domain in the DNS, causing the pressure differences there to be smaller  
 629 than predicted by the single column model. This could possibly be remedied by using a  $z$ -dependent  $\gamma$  parametrization,  
 630 which would fit well with the discussion of LES in section 2.2.1.

631 The two-fluid model keeps area fractions,  $\sigma_i(z)$ , close to 0.5. This is expected as the divergence-based transfer  
 632 is known to keep  $\sigma_i(z)$  roughly constant (Weller et al., 2020). In contrast, the area fractions diagnosed from the DNS  
 633 diverge from 0.5 either side of the centre (where symmetry demands equal fractions), reaching a maximum close to  
 634 the boundaries approaching 0.3 and 0.7.

### 635 | Transition to turbulence ( $Ra = 10^8$ )

636 Between  $10^7 < Ra \lesssim 5 \times 10^8$ , the DNS solutions transition from laminar flow to fully developed turbulence. The  
 637 buoyancy field of figure 1b is characteristic of this transitional regime. Besides the solutions becoming intermittent and  
 638 transient rather than (quasi-)periodic, the plume separation from the boundary layer fundamentally changes: above  
 639  $Ra \approx 10^7$ , regions of recirculation develop at the base of the plumes.

640 Results of a two-fluid single-column model with  $\hat{\gamma}_0 \approx 0.47$ ,  $C = 0$  are compared with those from the horizontally-  
 641 averaged DNS in Fig. 5. As with the  $Ra = 10^5$  results, the values of  $\hat{\gamma}_0$  and  $C$  were chosen to give the best qualitative  
 642 agreement for all profiles. Better prediction of the pressure differences between the fluids near the boundaries is  
 643 achieved by increasing  $\hat{\gamma}_0$  by a factor of  $\approx 2$ ; however this degrades the agreement of the mean pressure profile with  
 644 the DNS profile. This again suggests that  $\gamma$  should be a function of  $z$ , either directly or through dependence on other  
 645 properties of the flow, for instance the TKE.

646 Comparisons with the DNS reference profiles are mostly the same as for the laminar case, except that the addi-  
 647 tional mixing caused by the recirculation regions at the base of the plumes modifies the profiles in the near-boundary  
 648 regions. This has the most obvious effect on the buoyancy profiles within each fluid, which no longer overshoot, and  
 649 on the volume fraction profile, which is no longer monotonic. The lack of overshoots is reproduced by transferring  
 650 the mean buoyancy,  $C = 0$ , a suitable model for well-mixed turbulent flow. The detailed differences to the profiles  
 651 caused by these recirculation regions are however not reproduced by this simple parametrization: better representa-  
 652 tion of the mass exchanges  $S_{ij}$  is required. The recirculation is counter to the large-scale circulation, and hence is not  
 653 captured either by our arguments for the scaling of  $\gamma$ , or by the divergence-based mass transfer.

### 654 | Fully developed turbulence ( $Ra = 10^{10}$ )

655 Above  $Ra \approx 5 \times 10^8$ , the DNS flow is fully turbulent, exhibiting structures on many scales from the domain depth  
 656 down to the exceptionally thin boundary layers, shown in Figs. 1c-d for  $Ra = 10^{10}$ . The recirculations at plume base

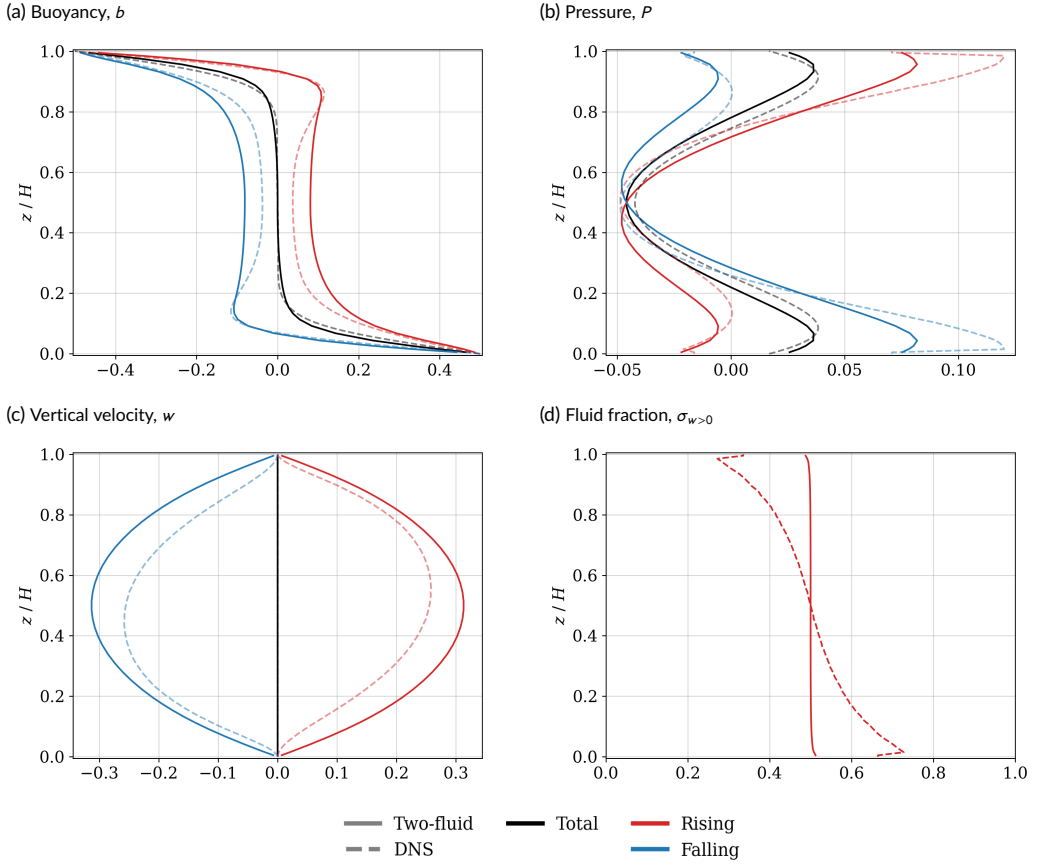


FIGURE 4 Two-fluid single-column model of  $Ra = 10^5$  RBC governed by equations (28)-(34) and (39), with closure constants  $\hat{\gamma}_0 \approx 0.75$ ,  $C = 0.5$ . Conditionally horizontally- and time-averaged profiles from the DNS are shown for reference.  $Nu = 7.1$ , reference  $Nu_{DNS} = 5.0$ .

657 first exhibited in the transitional regime divide into multiple small plumes which organize into a larger-scale circulation.  
 658 The bulk of the domain is statistically well-mixed.

659 Results from a two-fluid single-column model with  $\hat{\gamma}_0 \approx 0.44$ ,  $C = 0$  are shown in Fig. 6. Qualitative agreement  
 660 with the buoyancy and vertical velocity profiles is still good, but the mean pressure profile predicted by the model  
 661 now has too little curvature in the centre of the domain, and does not get the gradient correct close to the boundaries.  
 662 Again, the complex mixing of the turbulent flow has strong effects on the volume fraction profile, causing the volume  
 663 fraction of rising (falling) fluid to be less than 0.5 close to the lower (upper) boundary.

664 These larger discrepancies between the DNS and the two-fluid model model are possibly because the  $w = 0$   
 665 interface is now very complex. Figure 7 shows the  $w = 0$  interface superimposed on the DNS buoyancy fields at  
 666  $Ra = 10^8$  and  $Ra = 10^{10}$ . Although the dominant rising/falling two-fluid split is still into columns of falling and rising  
 667 air with an approximately vertical interface even in the higher  $Ra$  case, the simple split is increasingly complicated by  
 668 the complex vortical motions in the bulk of the fluid, and especially close to the base of the plumes. The intricate  
 669 dynamics of these interfaces are not accounted for by our single-column model.



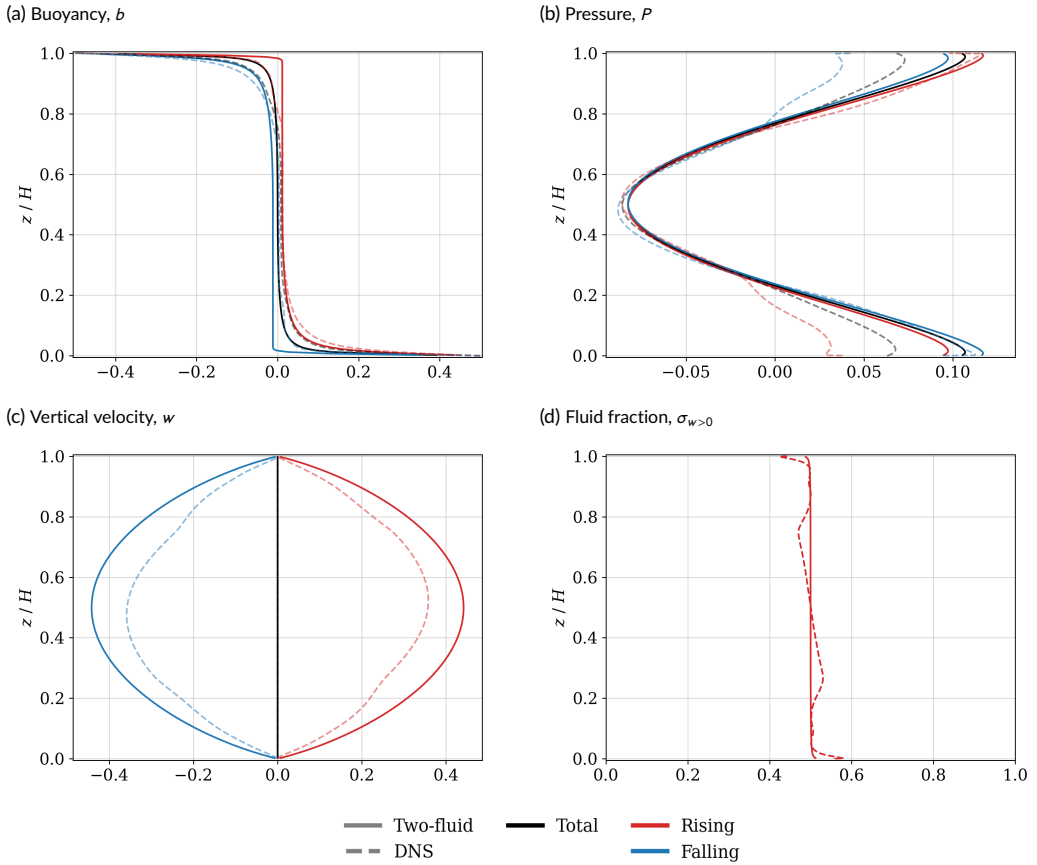


FIGURE 5 Two-fluid single-column model of  $Ra = 10^8$  RBC governed by equations (28)-(34) and (39), with closure constants  $\hat{\gamma}_0 \approx 0.47$ ,  $C = 0$ . Conditionally horizontally- and time-averaged profiles from the DNS are shown for reference.  $Nu = 41.6$ ; reference  $Nu_{DNS} = 27.9$ .

670 While there are quantitative discrepancies, for all three Rayleigh numbers the overall the agreement between  
 671 horizontally-averaged DNS and the two-fluid single-column model is good. Approximately the correct profiles are  
 672 captured even in the highly turbulent regime of  $Ra = 10^{10}$ . The model performs remarkably well given it has no repre-  
 673 sentation of sub-filter variability beyond the two-fluid split, showing that the model captures the essential coherent  
 674 overturning structures of Rayleigh-Bénard convection in all three characteristic regimes.

## 675 5.2 | Sensitivity to $\hat{\gamma}_0$ and $C$

676 In this section, the sensitivity of the model to the dimensionless closure parameters  $\hat{\gamma}_0$  and  $C$  is investigated. The  
 677 effects of changing  $\hat{\gamma}_0$  and  $C$  are similar at all Rayleigh numbers, so for brevity only  $Ra = 10^5$  is presented.

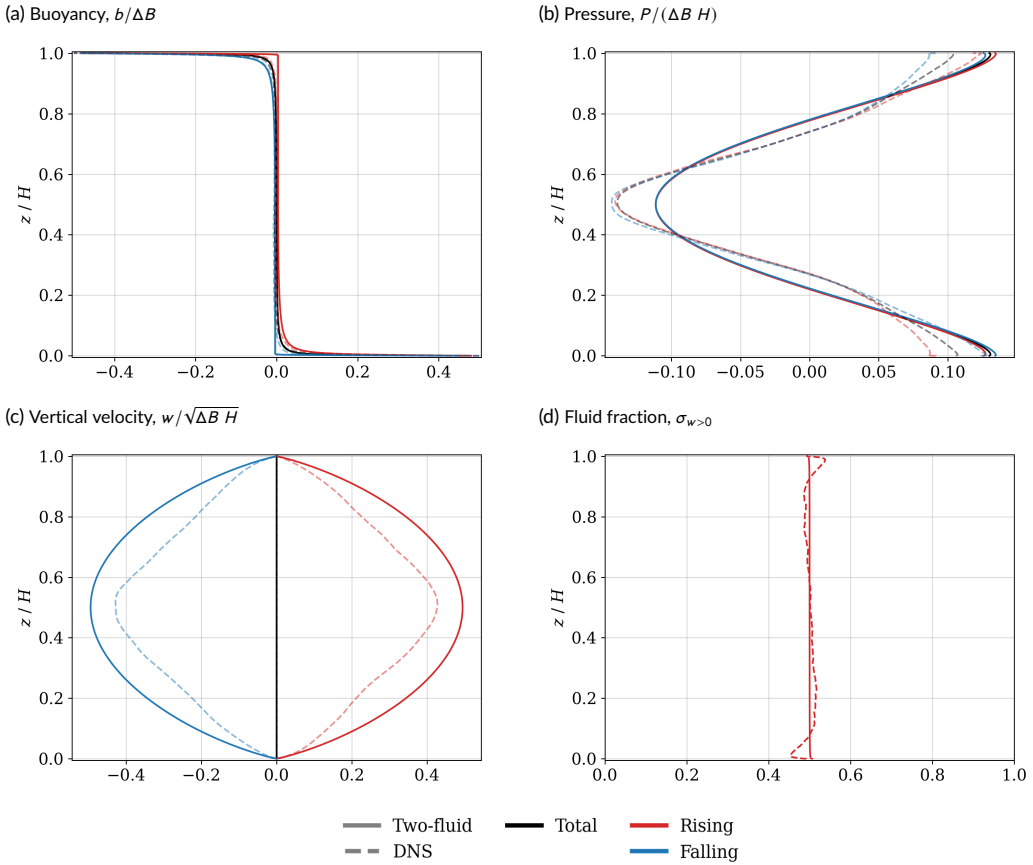


FIGURE 6 Two-fluid single-column model of  $Ra = 10^{10}$  RBC governed by equations (28)-(34) and (39), with closure constants  $\hat{\gamma}_0 \approx 0.44$ ,  $C = 0$ . Conditionally horizontally- and time-averaged profiles from the DNS are shown for reference.  $Nu = 228$ ; reference  $Nu_{DNS} = 94.5$ .

678 **5.2.1 | Sensitivity to  $\gamma$**

679 Figure 8 shows the effect on the two-fluid single-column steady-state of varying  $\hat{\gamma}_0$  from  $10^{-1} \lesssim \hat{\gamma}_0 \lesssim 10^1$ , along with  
 680 examples in the asymptotically-large and -small  $\hat{\gamma}_0$  regimes. The experiments were performed with  $C = 0.5$  at fixed  
 681  $Ra = 10^5$ , but the results are similar for all  $Ra$ .

682 The best qualitative match between the single-column and DNS profiles is found when  $\hat{\gamma}_0 \approx 0.75$ , as discussed  
 683 earlier, while the correct heat flux is predicted at  $\hat{\gamma}_0 \approx 1.861$ . These values are both  $O(1)$ , as expected. Agreement  
 684 with the reference profiles degrades sharply as  $\hat{\gamma}_0$  moves away from this range.

685 Increasing  $\hat{\gamma}_0$  increases the buoyancy difference between the fluids, and damps the vertical velocities – which  
 686 makes sense since in 1D this parametrization of  $p_i$  is similar to diffusion of the vertical velocity within a fluid, even  
 687 though the sum correction means no extra viscous term is added to the mean momentum budget. This effect is  
 688 already clear at  $\hat{\gamma}_0 = 2$ , where the vertical velocities are only  $\approx 2/3$  of those in the DNS, and the pressure profile  
 689 is much shallower, though still with the correct number of turning points. By  $\hat{\gamma}_0 = 10$ , the pressure profile loses the

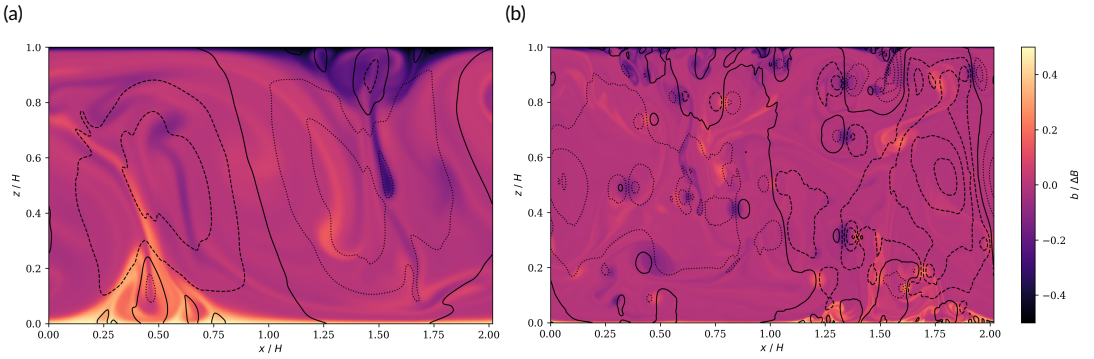


FIGURE 7 Snapshots of DNS buoyancy fields with overlaid vertical velocity contours at  $Ra = 10^8$  (a) and  $Ra = 10^{10}$  (b). Dashed contours denote  $w > 0$ , dotted  $w < 0$ , and the solid contour denotes  $w = 0$ . Contours above and below  $w = 0$  are spaced at intervals of  $U_B/4$ .

690 minimum in the centre of the domain, and the vertical velocities are almost zero. At asymptotically large  $\hat{\gamma}_0$ , the system  
 691 becomes subcritical and the solution is purely diffusive.

692 Decreasing  $\hat{\gamma}_0$  rapidly increases the pressure gradient, and deepens the minimum of the mean pressure in the  
 693 centre of the domain. This drastically increases the vertical velocities — by  $\hat{\gamma}_0 = 10^{-1}$ , the maximum vertical velocities  
 694 are over three times those of the DNS, and over twice those of the simulations with  $\hat{\gamma}_0 = 0.75$  discussed in detail earlier.  
 695 Decreasing  $\hat{\gamma}_0$  further only slightly changes these results, as seen for the asymptotically-small case of  $\hat{\gamma}_0 = \times 10^{-5}$ .

## 696 5.2.2 | Sensitivity to $C$

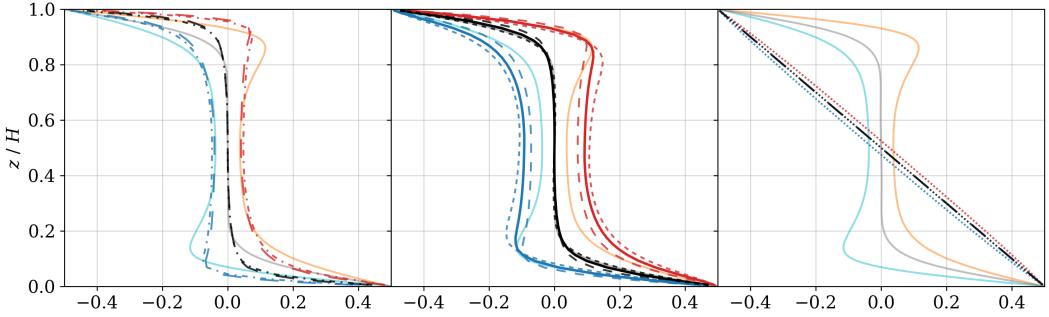
697 Figure 9 shows the steady-state effect of varying  $C$  from 0 (mean buoyancy is transferred:  $b_{ij}^T = b_i$ ) to 1 (zero buoyancy  
 698 is transferred over most of the domain:  $b_{ij}^T = 0$  wherever  $b_i = |b_i|$ ). Transfers with  $C > 1$  amount to transferring  
 699 buoyancies with magnitude greater than  $\Delta B$  close to the boundaries, which causes the solution to become unstable  
 700 at  $C \approx 1.3$ .

701 The main effect of increasing  $C$  is to generate the aforementioned overshoots in the within-fluid buoyancy pro-  
 702 files; this also steepens the pressure gradient, deepens the central pressure, and increases the magnitude of the  
 703 vertical velocities in each fluid. These effects are small compared to the order-of-magnitude effects associated with  
 704 varying  $\hat{\gamma}_0$ : for example, the maximum velocity increases monotonically from 0.3 to 0.45 as  $C$  increases from 0 to 1.  
 705 These effects are qualitatively similar at all  $Ra$ , but for  $Ra \gtrsim 10^7$ , the individual fluid buoyancy profiles no longer exhibit  
 706 overshoots, so  $C = 0$  provides a better fit with the DNS buoyancy profiles.

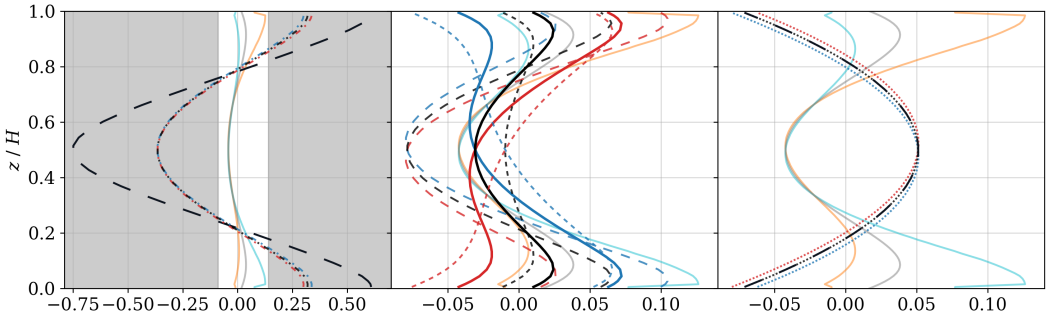
## 707 5.3 | Scaling of Nusselt and Reynolds numbers with Rayleigh number

708 To investigate the performance of the two-fluid single column model more systematically, the scaling of the Nusselt  
 709 number for single-column models across the Rayleigh number range  $10^2 \leq Ra \leq 10^{10}$  is compared with the DNS  
 710 results. The scaling  $\gamma/\nu \propto Ra^{1/4}$  (section 3.2) is evaluated, along with two choices of the transferred buoyancy,  $C = 0$   
 711 and  $C = 0.5$ . For each transferred buoyancy, the dimensionless proportionality factor  $\hat{\gamma}_0$  was fixed by finding the value  
 712 which gave the correct Nusselt number at  $Ra = 10^5$ . Fixing this constant at different Rayleigh numbers changes the

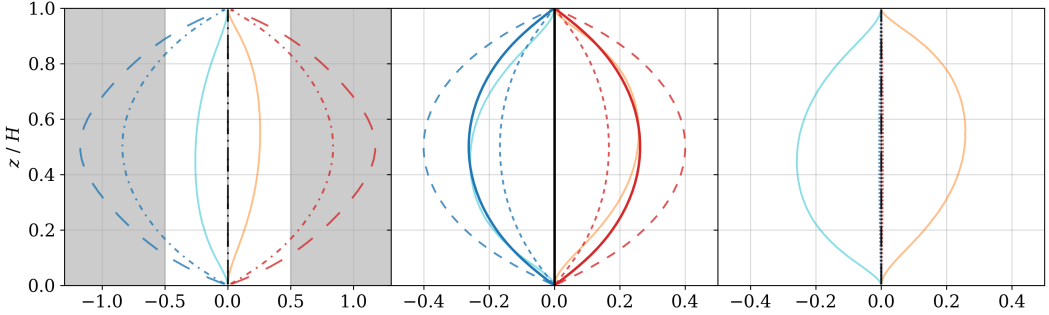
(a) Buoyancy,  $b/\Delta B$



(b) Pressure,  $P/(\Delta B H)$

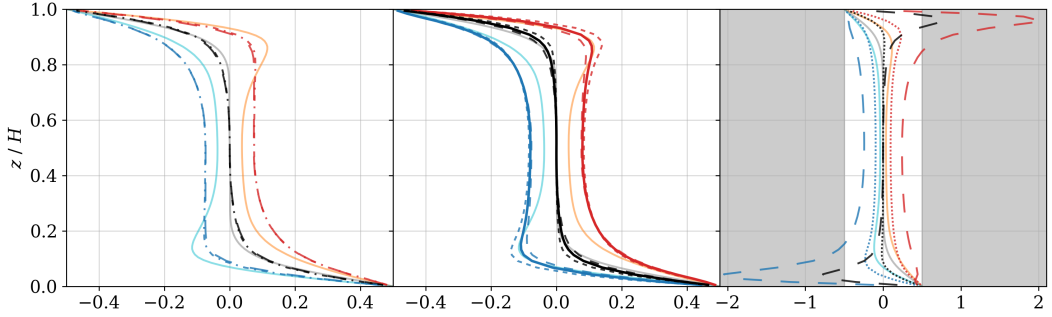
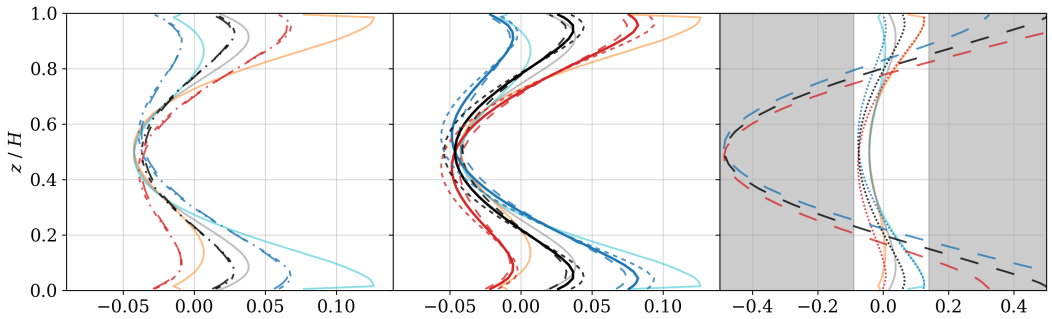
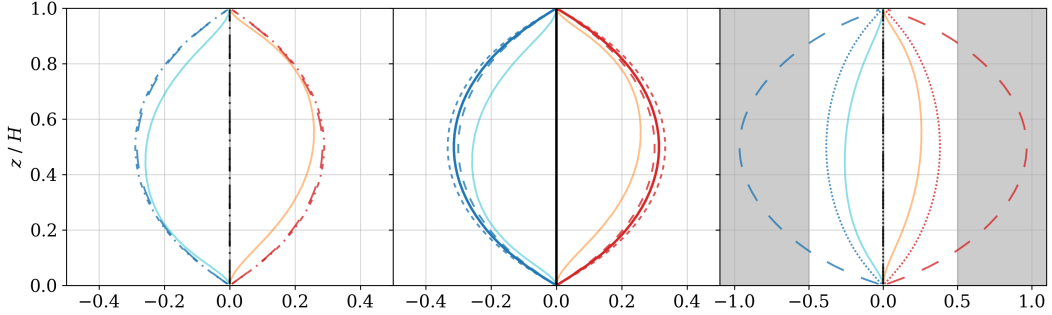


(c) Vertical velocity,  $w/\sqrt{\Delta B H}$



<span style="color: orange;">—</span> Rising (DNS)	<span style="color: red;">—</span> Rising (two fluid)	<span style="color: black;">—</span> $\hat{\gamma}_0 = 10^{-5}$	<span style="color: black;">- - -</span> $\hat{\gamma}_0 = 0.5$	<span style="color: black;">⋯</span> $\hat{\gamma}_0 = 10^1$
<span style="color: cyan;">—</span> Falling (DNS)	<span style="color: blue;">—</span> Falling (two fluid)	<span style="color: black;">- · - ·</span> $\hat{\gamma}_0 = 10^{-1}$	<span style="color: black;">—</span> $\hat{\gamma}_0 = 1$	<span style="color: black;">—</span> $\hat{\gamma}_0 = 10^5$
<span style="color: grey;">—</span> Total (DNS)	<span style="color: black;">—</span> Total (two fluid)		<span style="color: black;">- - -</span> $\hat{\gamma}_0 = 2$	

FIGURE 8 Two-fluid single-column model of  $Ra = 10^5$  RBC governed by equations (28)-(34) and (39), with  $C = 0.5$ , showing sensitivity to  $\hat{\gamma}_0$  (defined in eq. (39)) over the range  $10^{-1} \leq \hat{\gamma}_0 \leq 10^1$ . Profiles in the limit of asymptotically large ( $10^5$ ) and small ( $10^{-5}$ )  $\hat{\gamma}_0$  are also shown for reference.  $\hat{\gamma}_0 = O(1)$  is expected based on the scale analysis of section 3.2. Small values of  $\hat{\gamma}_0 (\leq O(10^{-1}))$  are shown in the left column, values of order 1 in the middle column, and large magnitudes ( $\geq O(10)$ ) in the right column. Grey shaded regions in plots in the left column highlight areas which are not in the domain of plots in the centre and right columns.

(a) Buoyancy,  $b/\Delta B$ (b) Pressure,  $P/(\Delta B H)$ (c) Vertical velocity,  $w/\sqrt{\Delta B H}$ 

— Rising (DNS)    — Rising (two fluid)    —  $C = 0$     - - -  $C = 0.3$     ⋯  $C = 1.0$   
— Falling (DNS)    — Falling (two fluid)    - - -  $C = 0.1$     - - -  $C = 0.5$     —  $C = 1.3$   
— Total (DNS)    — Total (two fluid)    - - -  $C = 0.7$

FIGURE 9 Two-fluid single-column model of  $Ra = 10^5$  RBC governed by equations (28)-(34) and (39), with  $\gamma_0 \approx 0.75$ , showing sensitivity to the transferred buoyancy parameter  $C$  (defined in eq. (33)) over the range  $0 \leq C \leq 1.3$ .  $C = 0.5$  corresponds to the profiles in figure 4. For  $C \geq 1.3$ , the solution becomes unstable. Results for small values of  $C$  ( $= 0, 0.1$ ) are shown in the left column; for values around the central value of 0.5 in the middle column; and for large values ( $\geq 1$ ) in the right column (see text for interpretation). Grey shaded regions in plots in the right column highlight areas which are not in the domain of plots in the left and centre columns.

713 prefactor of the  $Nu(Ra)$  scaling, but does not change the scaling itself.

714 Figure 10a shows  $Nu$  against  $Ra$  for the different values of  $C$  and scalings for  $\gamma$ . The DNS results are shown for  
 715 comparison, along with results from the single column model run with both tunable parameters set to zero,  $C = \hat{\gamma}_0 = 0$ .  
 716 All models with  $\hat{\gamma}_0 > 0$  perform significantly better than the model with  $\hat{\gamma}_0 = 0$ , which becomes supercritical for  
 717  $Ra < 10^3$  and follows a  $Nu(Ra)$  scaling with exponent everywhere  $> 0.33$ .

718 Models with  $\gamma/\nu \propto Ra^{1/4}$  show exceptional agreement with the DNS heat fluxes for  $Ra \geq 10^4$ , giving  $Nu \sim Ra^{2/7}$   
 719 with both  $C = 0$  (green curve) and  $C = 0.5$  (purple curve). This shows that the Nusselt number scaling exponent  
 720 depends on  $\gamma/\nu$  but not on  $C$ ; this makes sense since  $C$  is a crude parametrization for *how* the flow produces a given  
 721 heat flux, and should not affect the scaling of the heat flux itself. Below  $Ra = 10^4$ , the models with different values of  
 722  $C$  produce slightly different behaviour: the  $C = 0$  solutions become supercritical below  $Ra = 10^3$ , inconsistent with  
 723 the known  $Ra_c \approx 1708$ . While the  $C = 0$  simulations are still subcritical at  $Ra = 10^3$ , the heat flux at  $Ra = 2 \times 10^3$   
 724 is roughly 30% too high. These discrepancies suggest that the scaling used for  $\gamma/\nu$  is not quite correct in the low  $Ra$   
 725 regime; unsurprising since the scaling argument assumed  $Re \gg 1$ . For the intended application to highly turbulent  
 726 atmospheric convection, however, this does not present a severe problem.

727 The single-column model does not naturally capture the drop in the prefactor of the Nusselt number scaling  
 728 which occurs as the flow transitions to turbulence around  $Ra \approx 10^7$ . The drop in the Nusselt number scaling prefactor  
 729 may not be a robust feature of the convective flow, so it is far more important to get the scaling exponent correct.  
 730 Such drops in the scaling prefactor are found in other RBC experiments (see Johnston and Doering, 2009; Roche  
 731 et al., 2004, for a 2D numerical and a 3D experimental example, respectively), but appear to be dependent directly  
 732 on the nature of the flow, rather than global in nature like the scaling exponent. However, this drop *can* be accurately  
 733 reproduced by using  $C = 0.5$  for  $Ra \leq 10^7$  and  $C = 0$  for  $Ra > 10^7$ , retaining the value of  $\hat{\gamma}_0 \approx 1.861$ . With this  
 734 parametrization, the Nusselt number is correctly predicted to within 5% across six orders of magnitude of buoyancy  
 735 forcing,  $10^4 \leq Ra \leq 10^{10}$ , and approximately the correct transitional behaviour is found for  $Ra < 10^4$ . This could be  
 736 diagnostically incorporated into the parametrization by, for instance, reducing  $C$  to 0 whenever the vertical velocity  
 737 maximum gives a turbulent  $Re \gtrsim 2 \times 10^3$ .

738 The Reynolds number in the single-column simulations was estimated from the maximum magnitude of the verti-  
 739 cal velocity; this should scale with the large-scale circulation, so makes sense for a bulk Reynolds number. The scaling  
 740 behaviour of the Reynolds number is also well-captured (figure 10b), in particular giving the same scaling exponent as  
 741 the DNS. Notably, the change in  $C$  required to capture the correct behaviour of  $Nu$  does not cause a corresponding  
 742 kink in the Reynolds number scaling. This suggests that  $C$  really is just a crude measure of the flow state. Future  
 743 work would hope to capture these flow states dynamically through representing the sub-filter scale variability of the  
 744 variables within each fluid.

## 745 6 | SUMMARY, CONCLUSIONS, AND FUTURE WORK

746 In this paper we have shown that the simple two-fluid single column model (28)-(34) can qualitatively reproduce  
 747 horizontal-mean DNS buoyancy, vertical velocity, and pressure profiles in all three characteristic regimes of Rayleigh-  
 748 Bénard convection. A scaling argument for the pressure differences between the fluids allows the model to predict  
 749 the correct power-law scaling of  $Nu \sim Ra^{2/7}$ , and after measuring a dimensionless constant at one Rayleigh number  
 750 the magnitude of  $Nu$  can be predicted to within 5% over 6 orders of magnitude of  $Ra$ . The model also captures  
 751 approximately the correct spin-up behaviour, and approximately the correct critical Rayleigh number. The closure  
 752 set is minimal, requiring only two constants to be set; and not finely-tuned, as both closure constants may be varied

753 significantly from their central values without destroying the solution.

754 Although we use a similar equation set and identical fluid definitions to Weller et al. (2020), this is the first such  
755 study to model a fully turbulent regime with these fluid definitions. It is also the first multi-fluid convection study to  
756 considerably vary the applied forcing, testing the robustness of the parametrization.

757 This demonstrates the essential validity of the multi-fluid concept: the model directly captures the dominant  
758 overturning circulation of convection, present even in the fully turbulent regime, by allowing for a circulation even in  
759 a single column. It is important to note that this performance is achieved without even a minimal treatment of fluxes  
760 due to variability within each fluid (i.e. conventional “turbulent” or “subfilter” fluxes) apart from the fixed viscosity and  
761 Prandtl number of the fluid.

762 With the current model the mean buoyancy profile (and therefore the Nusselt number), the vertical velocity max-  
763 ima in each fluid (and therefore the implied Reynolds number), and the pressure profile, cannot all simultaneously have  
764 the correct magnitude. It is unclear whether this is due to neglected subfilter variability (in the form of exchanged  
765 buoyancy or neglected subfilter stresses, for example), or due to inadequate representation of the fluid fraction trans-  
766 fers. A more accurate and flexible representation of these transfers is essential to progressing beyond single-column  
767 modelling.

768 Future work will test the two-fluid model of this paper in the grey zone of RBC, investigating how the closures  
769 scale with resolution, and noting what flow features are missed by the simple closures in a higher dimensional setting.  
770 Improvements could arise from a partition which better selects the coherent structures, and from representation  
771 of within-fluid variability by consideration of higher moments of the flow. In particular, DNS data may be used to  
772 diagnose  $S_{ij}$ ,  $b_{ij}^T$ ,  $u_{ij}^T$  for various filter scales and fluid definitions. Possible closures could be informed by direct analysis  
773 of the interactions between coherent structures, boundary layers, and homogeneous, isotropic bulk (Togni et al., 2015;  
774 Berghout et al., 2021).

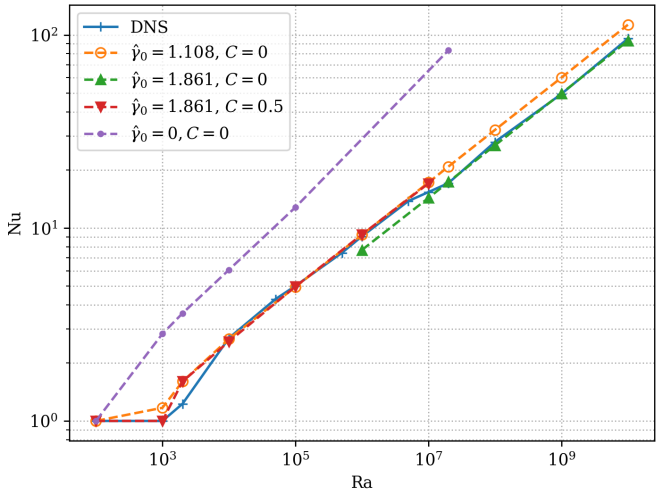
775 All of the above will develop fundamental understanding of the multi-fluid equations for convection. A thorough  
776 understanding of the dry convective grey zone, and of possible multi-fluid approaches to its parametrization, will help  
777 sharpen the questions for the much thornier problem of moist convection.

## 778 **acknowledgements**

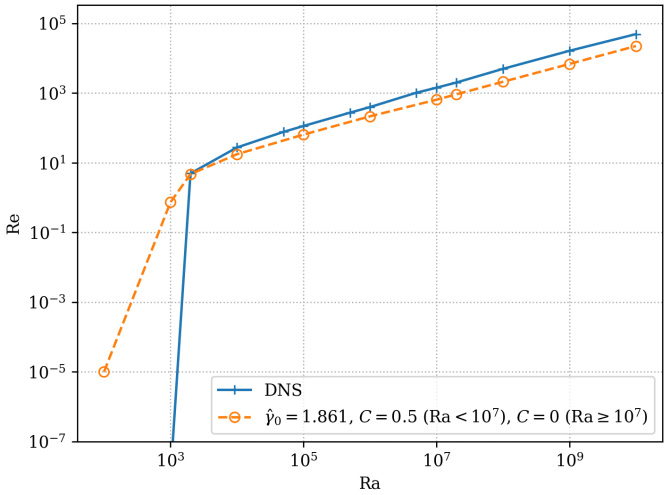
779 All authors acknowledge and thank the NERC/Met Office ParaCon project (grants NE/N013735/1, NE/N013743/1,  
780 NE/T003871/1, and NE/T003863/1) for funding this work. Simulations were performed using solvers from the At-  
781 mosFOAM ([github.com/AtmosFOAM/AtmosFOAM](https://github.com/AtmosFOAM/AtmosFOAM)) and AtmosFOAM-multiFluid ([github.com/AtmosFOAM/AtmosFOAM-](https://github.com/AtmosFOAM/AtmosFOAM-multiFluid)  
782 [multiFluid](https://github.com/AtmosFOAM/AtmosFOAM-multiFluid)) atmospheric computational fluid dynamics libraries, built on OpenFOAM-7 ([github.com/OpenFOAM/OpenFOAM-](https://github.com/OpenFOAM/OpenFOAM-7)  
783 [7](https://github.com/OpenFOAM/OpenFOAM-7)). Analysis of the data, and its manipulation for plotting, was made much easier by the OpenFOAM Python Parser  
784 ([pypi.org/project/Ofpp/](https://pypi.org/project/Ofpp/)) and PyFoam ([pypi.org/project/PyFoam/](https://pypi.org/project/PyFoam/)) Python packages.

## 785 **conflict of interest**

786 The authors declare no competing interests.



(a) Nusselt number vs. Rayleigh number for two fluid single column models with various values of  $\hat{\gamma}_0$  and  $C$ . The dashed blue curve shows the reference DNS results (as 2a), while the dashed brown curve shows the results of running the single column model with  $C = 0$  (mass exchanges transfer the mean buoyancy) and  $\gamma = 0$  (no pressure differences between the fluids). The green, purple, and red curves show the results for  $\gamma \sim Ra^{1/4}$ , with different values of  $\hat{\gamma}_0$ ; all give scalings of  $Nu \approx Ra^{2/7}$ . Single-column Nusselt numbers are calculated from the buoyancy gradient at the boundaries, and checked against the column-integrated buoyancy flux.



(b) Reynolds number vs. Rayleigh number for  $10^2 \leq Ra \leq 10^{10}$ . The dashed blue curve shows the reference DNS results (as 2b), while the solid orange curve shows results from a two fluid single column model obeying equations (28)-(34), with  $\gamma/\nu = 1.861 Ra^{1/4}$  and  $C = 0.5$  for  $Ra \leq 10^7$ ,  $C = 0$  for  $Ra > 10^7$ ; these constants give the best fit for  $Nu$  as a function of  $Ra$  (figure 10a). Both curves exhibit scalings of  $Re \approx Ra^{1/2}$  for  $Ra \geq 10^4$ . Single-column Reynolds numbers are calculated using the maxima of the individual fluid vertical velocity profiles for the velocity scale.

FIGURE 10



787 **references**

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