
¹ **Inertial effects on the vertical transport of suspended
2 particles in a turbulent boundary layer**

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⁶ **Abstract** In many atmospheric flows, a dispersed phase is actively suspended
7 by turbulence, whose competition with gravitational settling ultimately dic-
8 tates its vertical distribution. Examples of dispersed phases include snow, sea
9 spray droplets, dust, or sand, where individual elements of much larger density
10 than the surrounding air are carried by turbulent motions after emission from
11 the surface. In cases where the particle is assumed to deviate from local fluid
12 motions only by its gravitational settling (i.e. they are inertialess), traditional
13 flux balances predict a power law dependence of particle concentration with
14 height. It is unclear, however, how particle inertia influences this relationship,
15 and this question is the focus of this work. Direct numerical simulations are
16 conducted of turbulent open channel flow, laden with Lagrangian particles
17 of specified inertia; in this way the study focuses on the turbulent transport
18 which occurs in the lowest few meters of the planetary boundary layer, in re-
19 gions critical for connecting emission fluxes to the fluxes felt by the full-scale
20 boundary layer. Simulations over a wide range of particle Stokes number, while
21 holding the dimensionless settling velocity constant, are performed to under-
22 stand the role of particle inertia on vertical dispersion. It is found that particles
23 deviate from their inertialess behavior in ways that are not easily captured by
24 traditional theory; concentrations are reduced with increasing Stokes number.
25 Furthermore, a similarity-based eddy diffusivity for particle concentration fails
26 as particles experience inertial acceleration, precluding a closed-form solution
27 for particle concentration as in the case of inertialess particles. The primary

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consequence of this result is that typical flux parameterizations connecting surface emission models (e.g. saltation models or sea spray generation functions) to elevated boundary conditions may overestimate particle concentrations due to the reduced vertical transport caused by inertia in between; likewise particle emission may be underestimated if inferred from concentration measurements aloft.

Keywords atmospheric boundary layer · dispersion · dust · inertial particles · sea spray

1 Introduction

The planetary boundary layer (PBL) links the earth's surface to the atmosphere, and as a result controls the transmission of dust, salt, and other aerosols from their emission source at the surface to the larger meso- and synoptic-scale motions which govern their long-range transport and ultimate fate. Once airborne, these particulates can alter key chemical (O'Dowd and de Leeuw, 2007), optical (Kleefeld et al., 2002), and meteorological (Rosenfeld et al., 2008) processes before being deposited back onto the terrestrial or marine surface. Thus much work has been done in understanding and accurately parameterizing near-surface particle emission and transport processes for use in weather and climate prediction models, however continued discrepancies between models and observations remain a challenge (Knippertz and Todd, 2012; Reid et al., 2006). For instance the aircraft observation of large (up to 300 μm) sand grains above the Saharan Desert (Rosenberg et al., 2014) is in seeming contradiction with the upper limit of standard saltation models (Kok, 2011).

The difficulty of developing dust and aerosol emission schemes is due largely to unresolved, small-scale, and process-specific details, such as those resulting from wave breaking (Lewis and Schwartz, 2004) or saltation (Anderson and Haff, 1988). In this regard, the present work focuses on understanding the details of turbulent particle transport within the surface layer of the PBL — in particular the vertical flux of large particles which are heavy (i.e. they experience gravitational settling) and inertial (i.e. they do not necessarily follow fluid streamlines). It is the latter consideration, that of particle inertia, which is often neglected in particle flux parameterizations since even large sand grains or water droplets do indeed appear inertialess relative to PBL-scale motions. This work is focused, however, on turbulent transport which occurs in the lowest layers of the atmospheric surface layer (centimeters to meters above the surface), a region which plays the crucial role of connecting surface particle emission to transport throughout the full PBL, and where particle inertia can be non-negligible in their transport characteristics.

Attempts to parameterize heavy particle transport can begin by first approximating the suspended particulate as a passive scalar, in which case the horizontally-averaged vertical concentration profile and its relation to the surface flux could be described by Monin-Obukhov (MO) similarity theory (Monin

71 and Yaglom, 1971). The particles can be made more realistic by adding a
72 nonzero and constant settling velocity, which yields a power-law vertical pro-
73 file under neutral conditions when assuming that the turbulent diffusivity of
74 particle concentration is proportional to that of momentum (Prandtl, 1952;
75 Rouse, 1937), and reflects an equilibrium balance between suspension via tur-
76 bulence and gravitational settling. Other modifications, including disequilib-
77 rium between gravitational settling and turbulent suspension (Chamberlain,
78 1967; Kind, 1992), heterogeneous surface fluxes (Chamecki and Meneveau,
79 2011; Pan et al., 2013), non-neutral atmospheric stability (Freire et al., 2016),
80 or various other meteorological effects specific to, for instance, sea salt aerorols
81 (Toba, 1965) or snow (Pomeroy and Male, 1992), can be made as well.

82 It is well-known that particle inertia can lead to phenomena in turbulent
83 flows such as preferential clustering (Rouson and Eaton, 2001) or turbophoretic
84 drift (i.e. a net flux down a gradient of turbulent kinetic energy) (Reeks, 1983;
85 Sardina et al., 2012), and these play a key role in determining inertial particle
86 dispersion. For example, inhomogeneous horizontal particle distributions, such
87 as those found in sand streamers (Baas, 2008), may disrupt the assumptions
88 behind previous relationships. Much effort has gone into understanding inertial
89 particle transport in turbulent channel flows, relating particle dynamics with
90 turbulent events such as sweeps and ejections (Soldati and Marchioli, 2009;
91 Righetti and Romano, 2004) or studying the modulation of turbulence via the
92 suspended particles (Vreman, 2015), but many of these studies neglect the
93 effects of wall-normal gravitational settling. In the presence of gravitational
94 settling, particle clustering can lead to enhancements of the effective particle
95 settling velocity (Wang and Maxey, 1993; Aliseda et al., 2002), where the
96 average downwards particle velocity exceeds the still-air settling velocity as
97 predicted by, say, Stokes drag.

98 In the PBL, while many theoretical and computational attempts have been
99 made to characterize the Lagrangian dispersion characteristics of particles in
100 turbulence (Wang and Stock, 1993; Csanady, 1963), it remains unclear how
101 these effects of particle inertia modify the flux-profile relationship of particle
102 mass concentration in the PBL, particularly in the lowest layers near the sur-
103 face where Stokes numbers can be non-negligible. Even in theoretical studies
104 devoted to the topic of vertical particle dispersion which attempt to include
105 inertia, such as Belan et al. (2016), restrictions are necessarily made regarding
106 the degree of particle inertia and the regions of the flow where the corrections
107 are valid. Furthermore, in the well-known conceptual model for dry deposition
108 (Slinn and Slinn, 1980; Slinn, 1982), the overall deposition velocity of par-
109 ticulate matter is represented as a series of resistances to vertical transport,
110 including turbulence, molecular diffusion, and (when applicable) vegetative
111 canopies. This conceptual model is the basis for many studies which aim to
112 link surface emission to concentrations measured aloft — see for example Hop-
113 pel et al. (2002) or Fairall and Larsen (1984) — and within this framework
114 particle inertia is only occasionally considered (Zhang et al., 2001; Peters and
115 Eiden, 1992). When inertia is indeed included, it is only in the form of so-called
116 inertial impaction, the process by which particles can efficiently travel through

117 the diffusive sublayer due to inertia, thereby reducing the diffusive resistance
 118 to deposition.

119 The aim of the present study is to therefore investigate the role of parti-
 120 cle inertia on modifying concentration profiles and vertical fluxes in the first
 121 several meters of the PBL. This is done using an idealized approach based on
 122 direct numerical simulation (DNS), and focuses on the flux-profile relationship
 123 and potential modeling strategies. It is ultimately demonstrated that particle
 124 inertia can reduce turbulent fluxes of particle concentration, which can create
 125 a disconnect between true surface emission fluxes and fluxes felt by the full
 126 PBL. In some sense this is akin to an additional inertial resistance layer in
 127 the conceptual model of Slinn and Slinn (1980), and could potentially cause
 128 miscalculations of surface fluxes or overprediction of suspended particulate
 129 matter.

130 **2 Methodology**

131 **2.1 Numerical Simulation**

132 *2.1.1 Direct Numerical Simulation*

133 The basis of this study is DNS of turbulent open channel flow, where La-
 134 grangian particles are tracked individually. Details of the numerical method
 135 can be found in previous studies (Richter and Sullivan, 2013, 2014; Helgans and
 136 Richter, 2016), so only a brief summary will be included here. The neutrally-
 137 stratified, incompressible Navier-Stokes equations are solved in a Cartesian
 138 domain using a pseudospectral discretization in the homogeneous, periodic x
 139 and y directions and a second-order, finite difference discretization in the ver-
 140 tical, wall-normal z direction. Time integration is done via a low-storage, third
 141 order Runge-Kutta scheme (Spalart et al., 1991).

142 Mass and momentum conservation are given by:

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

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho_f} \frac{\partial p}{\partial x_i} + \nu_f \frac{\partial^2 u_i}{\partial x_j^2}, \quad (2)$$

143 where u_i is the fluid velocity, ρ_f is the fluid density, and ν_f is the fluid kine-
 144 matic viscosity. Incompressibility is enforced by solving a pressure Poisson
 145 equation at each Runge-Kutta stage. A no-slip condition is imposed at the
 146 lower domain wall, and a no-stress condition is imposed at the upper wall. The
 147 horizontal directions are periodic, and the flow is driven by a constant pres-
 148 sure gradient, chosen to produce turbulent open channel flow with a Reynolds
 149 number of $Re_* = 300$, where $Re_* = u_* H / \nu_f$ is the friction Reynolds number
 150 based on the domain height H and the friction velocity $u_* = \sqrt{\tau_w / \rho_f}$ (τ_w is
 151 the wall stress).

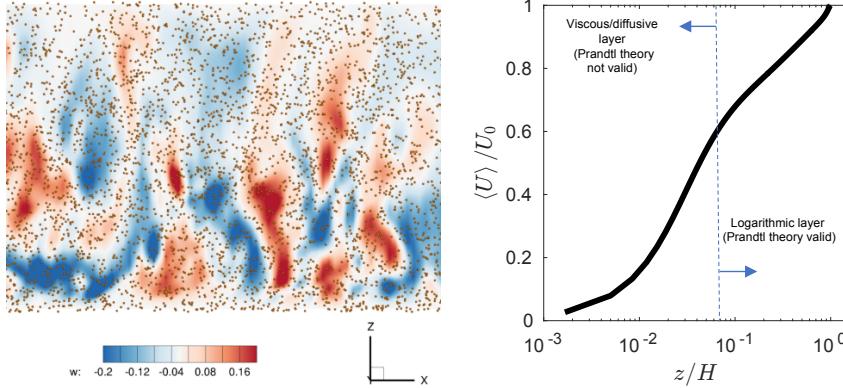


Fig. 1 Left: Snapshot of the computation. Colors reflect contours of fluctuating vertical velocity and brown dots represent Lagrangian particles. z axis in this figure has been magnified by a factor of 2.5. Right: mean velocity profile, showing the existence of a logarithmic layer above $z/H \approx 0.1$.

153 At the same time, an advection-diffusion equation for a passive scalar is
 154 computed as well:

$$\frac{\partial C}{\partial t} + \frac{\partial}{\partial x_j} (v_j C) = \Gamma_C \frac{\partial^2 C}{\partial x_j^2}, \quad (3)$$

155 where Γ_C is the molecular diffusivity of scalar C . The concentration is advected
 156 by a velocity v_j , which is not necessarily equal to the local fluid velocity u_j .
 157 For instance, as done by Chamecki et al. (2009), this can be set to $v_j =$
 158 $u_j - w_s \delta_{j3}$ to represent uniform gravitational settling, where $w_s = \tau_p g$ is the
 159 single-particle particle terminal velocity specified by its inertial time constant
 160 τ_p and the gravitational acceleration magnitude g , and δ_{j3} is the Kronecker
 161 delta. A truly passive scalar would have $v_j = u_j$. In this study we assume a
 162 Schmidt number $Sc = \nu_f / \Gamma_C$ of unity. At the lower boundary, the Dirichlet
 163 condition $C \equiv C_0 = 1$ is held fixed, while at the upper boundary a no-flux
 164 condition is imposed. The domain is initialized with $C = 0$ at $t = 0$.

165 *2.1.2 Lagrangian Particle Tracking*

166 The primary goal of this study is to characterize the effects of particle inertia
 167 on turbulent fluxes and vertical concentration profiles in a turbulent boundary
 168 layer, and this is readily accomplished using Lagrangian methods (see e.g.
 169 Balachandar (2009)). Thus each simulation is seeded with a large number of
 170 Lagrangian point particles, whose ensemble-averaged concentration field is the
 171 scalar C governed by Eq. 3. The particles are assumed to be one-way coupled,
 172 in that they do not have any influence on the surrounding flow, since we
 173 assume here that the mass fraction of suspended particles is sufficiently low.
 174 In air suspended with solid or liquid particles, this approximation holds if the

mass loading is roughly 1% or below (Balachandar and Eaton, 2010). Each particle obeys momentum conservation according to:

$$\frac{dv_{p,i}}{dt} = \frac{1}{\tau_p} (u_{f,i} - v_{p,i}) - g\delta_{i3}, \quad (4)$$

where $v_{p,i}$ is the particle velocity, g is the magnitude of gravitational acceleration, and $\tau_p = \rho_p d_p^2 / 18\rho_f \nu_f$ is the Stokes time scale. In these expressions d_p is the particle diameter, $u_{f,i}$ is the fluid velocity interpolated to the particle location, and ρ_p is the particle density.

In the limit of inertialess particles (i.e. the Stokes number $St \rightarrow 0$, where $St = \tau_p/\tau_f$ and τ_f is a relevant flow time scale; here we use the Kolmogorov time scale τ_K), Eq. 4 is not solved and rather the particle velocity is simply equal to the local fluid velocity less its terminal velocity:

$$v_{p,i} = u_{f,i} - \tau_p g \delta_{i3} = u_{f,i} - w_s \delta_{i3}. \quad (5)$$

In the further limit of massless particles, in which case the particles would simply represent a discretized form of a continuous passive tracer field, the particle velocity is equal to the local fluid velocity: $v_{p,i} = u_{f,i}$.

Given the restriction to relatively low Reynolds numbers due to the use of DNS, molecular diffusion of both momentum and scalar C occurs in a non-negligible region near the walls. To provide equivalency between the Lagrangian representation (i.e. the particles) and the Eulerian field C , the particles are moved according to a combination of their advection velocity $v_{p,i}$ and a Brownian step chosen to provide a diffusivity Γ_C :

$$dx_{p,i} = v_{p,i} dt + \sqrt{2\Gamma_C} d\xi_i, \quad (6)$$

where $d\xi_i$ is a Weiner process representing Brownian motion. Numerically, advection is solved using the same RK3 method used for the flow, and at the end of each time step, a random jump is added to provide the diffusive jump. Figure 1 provides a snapshot of the flow simulation with instantaneous particle location.

As noted above, the Eulerian scalar concentration C is held fixed at $C_0 = 1$ at the bottom wall, and a no-flux condition is imposed at the top wall. For Lagrangian particles, the same conditions are enforced: at the top wall, this means that particles are elastically reflected, and at the bottom wall, a reservoir of a constant number of particles just below the surface is maintained whose concentration is defined as $C_0 = 1$. The mean concentration $\langle C \rangle$ is then computed from a Lagrangian point of view at a specific height by counting the particles in the horizontal slab with volume $L_x \times L_y \times \Delta z$ (where L_x and L_y are the domain extents in the x and y directions and Δz is the vertical grid spacing at a particular height z) and normalizing with the concentration/volume combination maintained just below the bottom surface. This method requires a sufficient number of particles for statistical convergence of the particle averages, and in this case the number of particles maintained in the lower reservoir was held at 1×10^4 (this leads to particle numbers in the domain of $O(10^6)$).

213 Figure 2(a) shows a comparison between the Eulerian (Eq. 3) and La-
 214 grangian prediction of $\langle C \rangle / C_0$ in the inertia-free case, for three different set-
 215 tling velocities. The settling velocities w_s are normalized by κu_* so that they
 216 reflect the settling tendency as compared to the strength of wall shear stress —
 217 in sediment transport literature this ratio is commonly referred to as the Rouse
 218 number (Rouse, 1937). Figure 2(a) demonstrates the equivalence between the
 219 Eulerian and Lagrangian particle treatment, including the adjustment of the
 220 advection velocity v_i in Eq. 3 by the settling velocity.

221 2.2 Existing theory

222 Following Prandtl (1952) (and many others since), the Reynolds decomposition
 223 $C = \langle C \rangle + c'$ can be introduced into Eq. 3, and after averaging the equations
 224 in absence of particle inertia and a net surface flux (e.g. Kind (1992)), one
 225 recovers a balance between turbulent suspension and gravitational settling:

$$\langle c' w' \rangle - \langle C \rangle w_s = 0 \quad (7)$$

226 If one then makes the assumption that the turbulent particle concentra-
 227 tion flux $\langle c' w' \rangle$ can be expressed with an eddy diffusivity, in analogy with
 228 momentum and passive scalars, Eq. 7 becomes:

$$-K_C \frac{d \langle C \rangle}{dz} - \langle C \rangle w_s = 0, \quad (8)$$

229 where K_C is an eddy diffusivity. In the neutral atmospheric surface layer,
 230 Monin-Obukhov similarity theory implies $K_C = \kappa u_* z$ since the turbulent flux
 231 $\langle c' w' \rangle$ does not vary with height (here $\kappa = 0.41$ is the von Kármán constant
 232 and the turbulent Schmidt number is assumed to be unity). For open channel
 233 flow, however, the linearly varying momentum flux with height results in a
 234 parabolic diffusivity profile, given by $K_C = \kappa u_* z (1 - z/H)$ (see for example
 235 Fischer (1973)).

236 In its original formulation, the Prandtl solution to the ordinary differential
 237 equation of Eq. 8 suggests that the average concentration varies as a power law
 238 with height, with an exponent of $w_s / (\kappa u_*)$. Using the open channel version
 239 of K_C yields an equivalent result for systems where the total momentum flux
 240 varies linearly with height, which is a product of two power laws:

$$\frac{\langle C \rangle(z)}{C_r} = \left(\frac{z}{z_r} \right)^{-w_s / \kappa u_*} \left(\frac{z - H}{z_r - H} \right)^{w_s / \kappa u_*} \quad (9)$$

241 Here, z_r is a constant reference height where the mean concentration is C_r
 242 ($z_r = 0.3H$ in this work). Throughout the manuscript, the “Prandtl” solution
 243 will refer to Eq. 9, although it represents a profile in an open channel config-
 244 uration where the eddy diffusivity K_C is parabolic with height, as opposed to
 245 the original atmospheric surface layer version (Prandtl, 1952). As noted previ-
 246 ously, throughout the literature (particularly in relation to sediment transport)
 247 this profile is also sometimes referred to as the Rouse profile (Rouse, 1937).

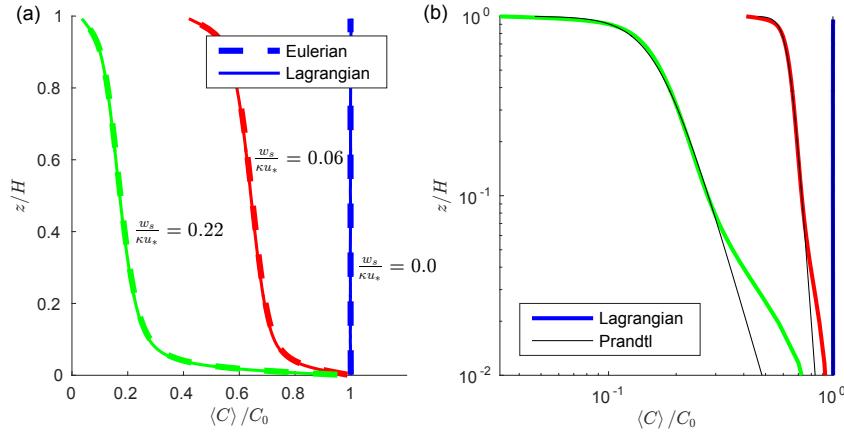


Fig. 2 Mean normalized particle concentration $\langle C \rangle / C_0$ versus normalized height z/H for three different settling velocities without inertia. Colors indicate different settling velocities and are indicated on the left. (a) Linear axes showing the comparison between the Eulerian solution (solid lines) and Lagrangian solution (dashed lines). (b) Logarithmic axes comparing the computed solutions to the Prandtl (1952) theory (Eq. 9).

248 Figure 2(b) shows that the Prandtl solution of Eq. 9 agrees very well with
 249 the concentration profiles computed in the inertialess cases, above a height
 250 of z/H around 0.1. Below this height, molecular diffusivity plays a large role
 251 (since the simulations are based on DNS), violating the basic assumption that
 252 the particle concentration is a result of a balance between turbulent suspen-
 253 sion and gravitational settling. Thus in the absence of particle inertia, Eq. 9
 254 accurately predicts concentrations over a range of settling velocities in regions
 255 of the flow where turbulence and gravity are indeed the dominant transport
 256 mechanisms.

257 3 Results and discussion

258 3.1 Interpretation

259 The numerical methodology outlined in the previous sections represents an
 260 idealized approach towards understanding the role of inertia in the flux-profile
 261 relationship of suspended particles. As such, we include here a brief discussion
 262 of both the applicability of the following results, as well as an explanation for
 263 how they should be interpreted.

264 First, the lower boundary conditions utilized for both the Eulerian and
 265 Lagrangian simulations are not intended to physically represent the process of
 266 particle emission from the surface. Since aeolian saltation at the sand/snow
 267 surface, droplet formation at the air-sea interface, lifting at the subaqueous
 268 sediment layer, etc. have widely varying physical explanations, the focus here
 269 is instead on the vertical transport of particles *once they have been suspended*.

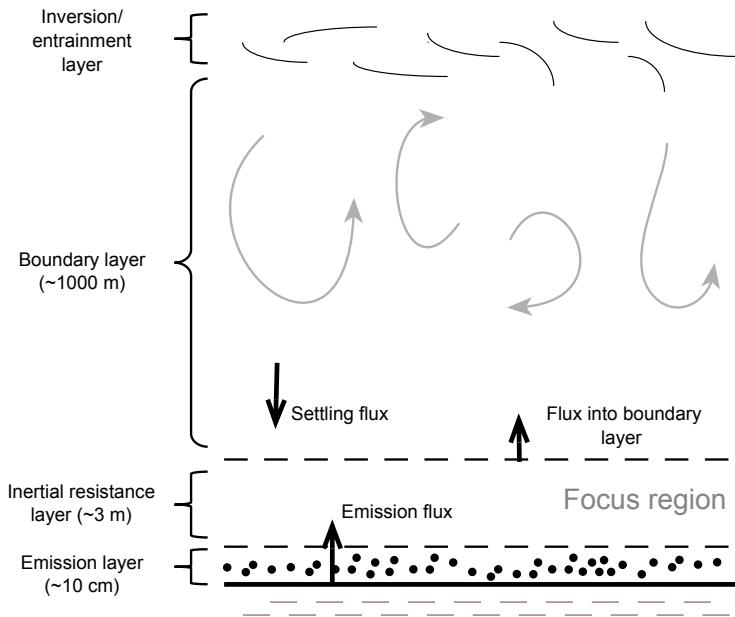


Fig. 3 Schematic detailing the structure of the PBL and the focus of the present DNS study. In the region above the emission layer and below the full boundary layer, local Stokes numbers can be large due to the rapid change in the turbulent kinetic energy dissipation rate with height, resulting in inertia-dominated transport of particles in the bottom few meters of the PBL. The emission layer includes the region where processes such as bubble bursting or saltation occur, which are not explicitly represented in this study.

270 In the present work, molecular diffusion, as represented by Brownian motion
 271 for the Lagrangian particles and by a constant molecular diffusivity for the
 272 Eulerian concentration field, is used as a means for achieving this suspension,
 273 in the sense that it is responsible for carrying particles from the specified
 274 concentration at the surface to a level where turbulence dominates transport
 275 (this occurs at a level of $z/H \approx 0.1$ in the DNS presented here). This allows
 276 for a direct comparison between the Eulerian and Lagrangian methods, and
 277 allows us to focus instead on the turbulent transport in regions above this
 278 layer. How the particles have arrived this this height is immaterial for our
 279 purposes.

280 Second, the DNS framework is meant to represent only the lowest few
 281 meters of the PBL where inertia is present (the “inertial resistance layer” —
 282 see Fig. 3). Thus the parameter H in the simulations is not the boundary layer
 283 height of $O(1000\text{ m})$ but rather the top of the inertial resistance layer which
 284 has a height of $O(1\text{ m})$. For a given particle size, the Stokes number computed
 285 based on the local Kolmogorov time scale changes very rapidly with height,
 286 leaving a region near the surface (but above the emission layer) where inertia

287 can be large. The depth of this layer is controlled by both the particle size
 288 and the turbulence levels in the boundary layer. Since $St = \tau_p/\tau_K$ depends
 289 on both τ_p and the local Kolmogorov time scale, the depth of this layer would
 290 scale as d_p^2 , since τ_p is proportional to d_p^2 , and with $u_*^{3/2}$, since the turbulent
 291 kinetic energy dissipation rate ϵ is proportional to u_*^3 and τ_K is proportional
 292 to $\epsilon^{-1/2}$ (at least in neutral conditions). As demonstrated below in section 3.6,
 293 the features observed in the DNS can be felt throughout larger-scale models
 294 which cannot resolve these small-scale motions and instead resolve PBL-scale
 295 motions.

296 3.2 Adding particle inertia

297 The goal of this work is to extend the analysis of section 2.2 to include par-
 298 ticles which exhibit appreciable inertia during their turbulent transport. In
 299 most studies on this topic (Chamberlain, 1967; Chamecki et al., 2009; Kind,
 300 1992), particle inertia is neglected and only gravitational settling is taken into
 301 consideration. In other studies (Belan et al., 2016; Csanady, 1963; Freire et al.,
 302 2016), particle inertia is treated insofar as it is responsible for altering disper-
 303 sion rates, and compared to the large scales associated with the full PBL the
 304 effect of inertia is quite small. Here, our focus is on the lowest layers of the
 305 particle-laden boundary layer, where the transport is crucial for linking the
 306 small-scale emission processes with the large-scale PBL.

307 With this in mind, we design a set of numerical experiments whose purpose
 308 is to systematically vary the particle inertia while holding the settling tendency
 309 the same, in order to determine the effects on the average concentration profiles
 310 and flux characteristics. A nondimensional settling velocity of $w_s/(\kappa u_*) = 0.06$
 311 is held fixed (red lines in Fig. 2), and the flow Reynolds number is likewise fixed
 312 at $Re_* = 300$. The particle inertial time scale τ_p is then varied to provide Stokes
 313 numbers ranging between $St = 0.05$ and $St = 5.0$. We note that the following
 314 analysis only reports results from a single nondimensional settling velocity, but
 315 the same general results are found at other values of $w_s/(\kappa u_*)$. The effect of
 316 w_s is to modify the baseline concentration profile, from which inertia modifies
 317 as described below. We also note that while holding w_s constant while varying
 318 St is artificial, it allows us to target explicitly the effects of inertia, without
 319 confounding them with changes in w_s at the same time. In reality, w_s and St
 320 are linked via τ_p , although local values of St can change with height.

321 For our DNS, we use a flow time scale of $\tau_f = \bar{\tau}_K$ to define St , where $\bar{\tau}_K$ is
 322 the vertically-averaged Kolmogorov time scale in the channel. For reference, if
 323 one uses the logarithmic scaling of viscous dissipation rate in the atmospheric
 324 surface layer, $\epsilon = u_*^3/\kappa z$, then $\bar{\tau}_K$ averaged over the lower 5 meters of the
 325 surface layer for $u_* = 0.4 \text{ m s}^{-1}$ is roughly 0.015 seconds. In these conditions
 326 the Stokes number range of $St = 0.5$ to $St = 5.0$ corresponds to diameters of
 327 $d_p \approx 10 \mu\text{m}$ to $d_p \approx 150 \mu\text{m}$ when the particle density is of order 1000 kg m^{-3} .
 328 Thus spray droplets or dust particles suspended in air can quite easily behave

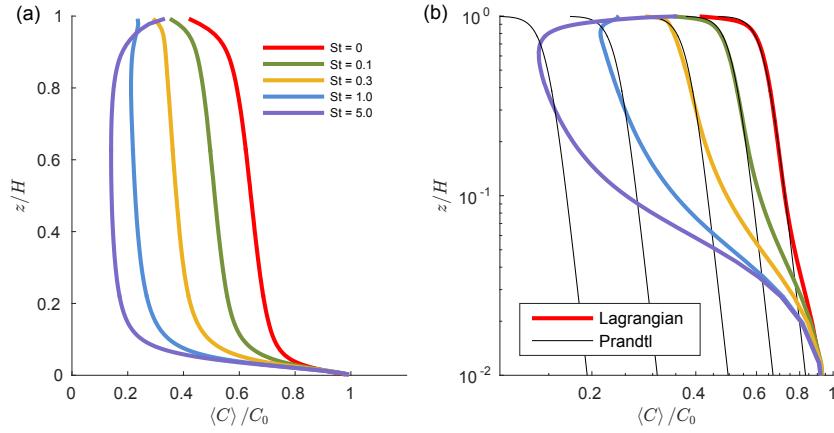


Fig. 4 (a) Average normalized concentration $\langle C \rangle / C_0$ computed from the inertial, Lagrangian simulations as a function of z/H . The settling velocity is held fixed at $w_s / (\kappa u_*) = 0.06$ for all cases, and $Re_* = 300$. (b) The same concentration profiles on logarithmic axes, with Eq. 9 plotted in thin black lines for reference. The addition of inertia dramatically changes the concentration within the domain, and causes the average profile to deviate significantly from the inertialess theory.

329 as inertial particles within $O(1\text{ m})$ of the surface (i.e. the ‘‘inertial resistance
330 layer’’ found in Fig. 3).

331 Figure 4(a) presents the normalized average concentration profiles as a
332 function of z/H over the range of St considered. Despite the settling velocity
333 being identical between these cases, the addition of inertia clearly inhibits
334 the ability of particles to distribute vertically throughout the domain. Over
335 the present range of St , this trend is monotonic, in that higher St leads to
336 lower mean concentrations throughout the entire channel. The exception is the
337 $St = 5.0$ case, where upwards turbophoretic drift (Reeks, 1983; Sardina et al.,
338 2012) actually overcomes gravitational settling, pushing particles towards the
339 top wall and increasing concentrations there (i.e. the finite size of the domain
340 begins to contaminate the solution since vertical velocity fluctuations must
341 approach zero at the top wall).

342 Figure 4(b) illustrates that the Prandtl theory describing the vertical pro-
343 files of concentration as a balance between turbulent flux and gravitational
344 settling fails significantly as St is increased (thin black lines). At low St , Eq. 9
345 is still accurate in the upper regions of the domain, but the height range over
346 which agreement is found diminishes. The disagreement propagates from the
347 bottom, since the local Stokes number, as computed by the local value of τ_K ,
348 is a monotonically decreasing function with height. Thus the first regions of
349 the flow where the theory begins to fail are those where the local St is locally
350 large enough to cause the particles to cease acting like settling, passive tracers.

351 By solving Eq. 3 and only considering gravitational advection (i.e. $v_j =$
352 $u_j - w_s \delta_{j3}$), the turbulent flux $\langle c' w' \rangle$, diffusive flux $-\Gamma_C (\partial \langle C \rangle / \partial z)$, and grav-
353 itational flux $-w_s \langle C \rangle$ are computed directly from the Eulerian concentration

354 field. Simultaneously, the same flux quantities can be computed from the La-
 355 grangian particles as well. The gravitational flux is still $-w_s \langle C \rangle$ (using the
 356 Lagrangian-based $\langle C \rangle$), and Reynolds averaging of the particle evolution equa-
 357 tions shows that the sum of the turbulent and gravitational fluxes is equal to
 358 $\langle w_p \rangle \langle C \rangle$, where $\langle w_p \rangle$ is the average particle vertical velocity. Therefore the
 359 turbulent flux (counterpart to $\langle c'w' \rangle$ in the Eulerian frame) is the difference
 360 between the gravitational flux and the concentration-weighted average particle
 361 velocity. Finally, the total flux is computed from the Lagrangian point of view
 362 by keeping track of the net number of particles crossing each horizontal plane
 363 in each time step. From this total, the gravitational and turbulent fluxes can
 364 be subtracted to yield the diffusive flux.

365 First, to demonstrate that the Eulerian versus Lagrangian-based flux calcu-
 366 lations are equivalent for systems with no inertia, Fig. 5 shows the Lagrangian-
 367 computed profiles in thick red lines and the Eulerian-computed fluxes thin
 368 black lines for the inertialess case shown in Figure 4. It is clear that the flux
 369 profiles in this case are nearly identical, and therefore the Lagrangian-based
 370 fluxes are accurate representations of vertical particle transport.

371 Several features are of note in Fig. 5. First, since we average only after
 372 the system has reached steady state, the total flux should be zero, which
 373 Fig. 5 indeed indicates is the case. Figure 5 shows that in this steady state
 374 condition, above $z/H \approx 0.1$ and below $z/H \approx 0.9$, the flux balance, even in the
 375 presence of substantial particle inertia, is strictly between gravitational settling
 376 and turbulent suspension. As expected, this spatial region corresponds to the
 377 region of Fig. 4 where the Prandtl-predicted concentration profile agrees with
 378 the simulations in the absence of particle inertia. Near the top and bottom
 379 walls, turbulent fluxes are replaced by nonzero diffusive fluxes, thus violating
 380 the assumptions behind the Prandtl theory.

381 Figure 5 also illustrates that within the regions unaffected by diffusion, in-
 382 creases in particle inertia suppress turbulent fluxes, which are in turn balanced
 383 by lower gravitational settling fluxes. So while the dominant balance remains
 384 between turbulence and gravity, their magnitudes have deviated sharply from
 385 the noninertial case. This trend increases with St , and the inertialess Eulerian
 386 formulation (thin black lines) is clearly insufficient in predicting the fluxes for
 387 inertial particles.

388 3.3 Inertial correction to the advection velocity

389 In order to capture inertial effects in the Eulerian calculations, we utilize an
 390 inertial correction to the advection velocity v_j in Eq. 3 which is based on an
 391 asymptotic expansion of equation 4 in Stokes number, retaining only the first
 392 order correction (Druzhinin, 1995; Maxey, 1987). More recent implementations
 393 of this correction have acquired the name of the “Equilibrium Eulerian” model,
 394 whose advantage is that it captures some inertial affects while still allowing
 395 the particle advection velocity to be written in terms of local flow velocities
 396 and accelerations (Ferry and Balachandar, 2001; Balachandar, 2009).

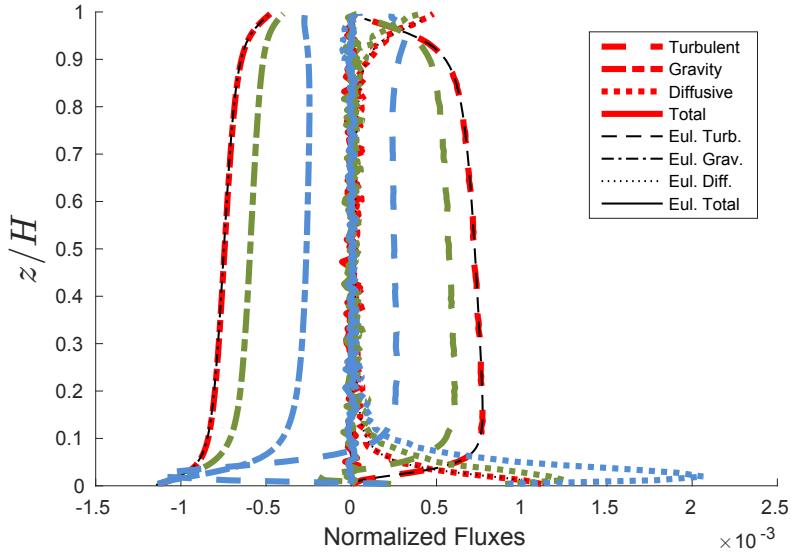


Fig. 5 Vertical profiles of concentration fluxes for a subset of the overall Stokes numbers: $St = 0$ (red), $St = 0.1$ (green), and $St = 1.0$ (blue). Line types provided in the legend refer to the turbulent flux, the gravitational flux, the diffusive flux, and the total flux. The thick colored lines refer to fluxes computed from the Lagrangian particle data; thin black lines are fluxes from an Eulerian, inertialess perspective. Fluxes normalized by $C_0 U_0$, where U_0 is the maximum velocity in the channel.

397 Under this approximation, the advection velocity takes the form:

$$v_j = u_j - w_s \delta_{j3} - \tau_p \frac{Du_j}{Dt}, \quad (10)$$

398 where $\frac{D}{Dt} = \frac{\partial}{\partial t} + u_k \frac{\partial}{\partial x_k}$ is the total fluid acceleration. The meaning of the last
 399 term in Eq. 10 is that the fluid velocity seen by the particle at a time τ_p before
 400 the present time should be factored into the current particle velocity due to
 401 inertia, and would only be expected to be accurate below $St \approx 0.2$ since the
 402 correction is only first order (Ferry and Balachandar, 2001).

403 Following the same Reynolds averaging procedure as done for deriving Eq.
 404 7, this correction to the advection velocity leads to two additional terms in
 405 the vertical flux balance:

$$\langle c' w' \rangle - \langle C \rangle w_s - \langle C \rangle \tau_p \frac{\partial \langle w'^2 \rangle}{\partial z} - \tau_p \left\langle c' \frac{Dw'}{Dt} \right\rangle = 0. \quad (11)$$

406 The first two terms are the same turbulent and gravitational settling fluxes
 407 from Eq. 7. The third term on the left hand side of Eq. 11 represents tur-
 408 bophoresis, where inertia causes a drift against gradients of turbulent kinetic
 409 energy (Reeks, 1983), and the fourth term on the left hand side represents
 410 correlations between concentration fluctuations and vertical accelerations. It

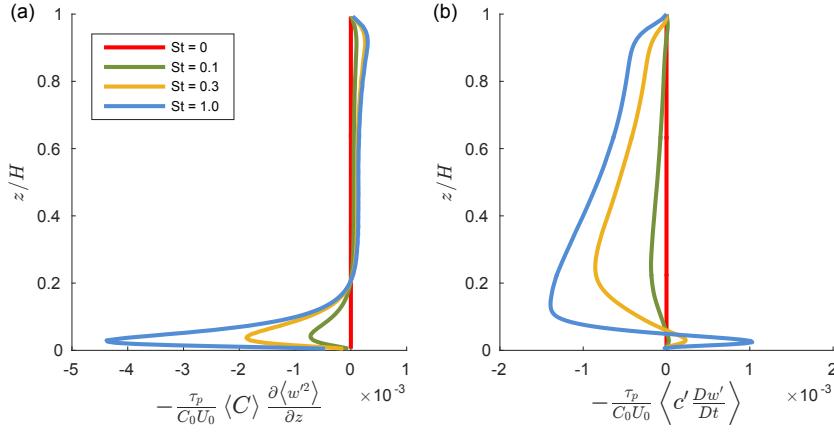


Fig. 6 Additional, inertia-based flux terms in Eq. 11 as a function of height. Different lines refer to different Stokes numbers ranging between 0 and 1.0 (see legend). (a) turbophoresis term: $-\tau_p \langle C \rangle \frac{\partial \langle w'^2 \rangle}{\partial z}$, (b) correlation between concentration fluctuations and vertical accelerations: $-\tau_p \langle c' \frac{Dw'}{Dt} \rangle$. Both terms normalized by $C_0 U_0$.

411 can be easily shown that the sum of these two terms is simply $-\tau_p \langle C \frac{Dw'}{Dt} \rangle$,
 412 i.e., the correlation of the total concentration with vertical acceleration.

413 With this formulation in mind, we perform a new simulation in which v_j
 414 in Eq. 3 is replaced by Eq. 10 in order to compare its predictions with the true
 415 behavior of the inertial Lagrangian particles (here “true” indicates that we
 416 expect the theory to match the Lagrangian simulations exactly if the theory
 417 were correct). From these calculations, Fig. 6 presents the two extra flux terms
 418 in Eq. 11 as a function of height for a range of St , which shows that each of
 419 the inertial corrections to the vertical flux are of the same order of magnitude.
 420 As expected, the turbophoretic term in Fig. 6(a) is largest in the regions near
 421 the lower wall where the gradients of the turbulent kinetic are the highest.
 422 These profiles are related to one another, in the sense that the gradient $\frac{\partial \langle w'^2 \rangle}{\partial z}$
 423 is the same in all cases since the underlying turbulence has not changed with
 424 particle Stokes number.

425 In the range where molecular diffusion is unimportant (above $z/H \approx 0.1$),
 426 the concentration fluctuation/vertical acceleration correlation term (Fig. 6(b))
 427 is dominant and negative, suggesting that inertia tends to reduce the vertical
 428 flux. This is in agreement with the Eulerian-based fluxes computed in Fig. 5,
 429 and provides an Eulerian interpretation of this suppression of the concentration
 430 flux. It is noteworthy that the dominance of this term over the turbophoretic
 431 term indicates that inertial corrections to vertical dispersion must include
 432 additional effects beyond turbophoretic drift. As the particle Stokes number
 433 increases, these flux corrections generally become larger since they are pro-
 434 portional to τ_p , although the correlation saturates around $St = 0.5$. We note
 435 that the corrections for $St = 5.0$ are not shown since the inertia-corrected ad-

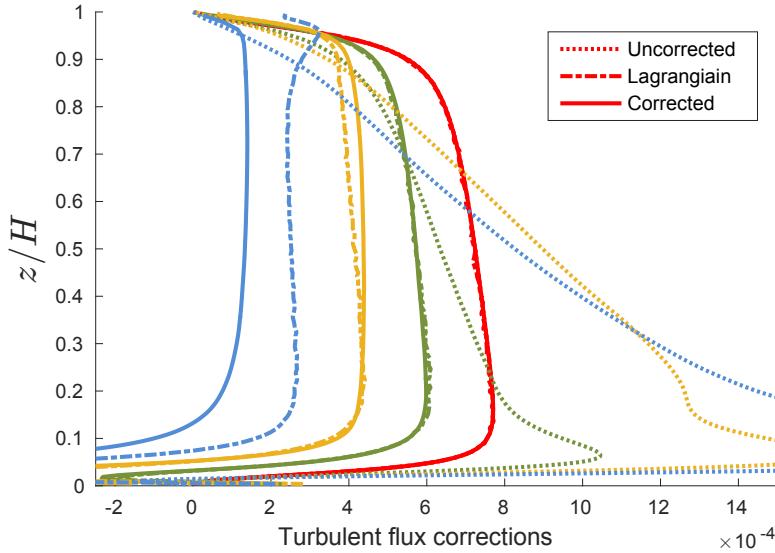


Fig. 7 Turbulent fluxes with inertial correction to Eulerian advection velocity. Uncorrected turbulent flux $\langle c'w' \rangle$ (dashed), Lagrangian turbulent flux (dash-dotted), and the corrected turbulent flux $\langle c'w' \rangle_{corr}$ (solid). Line colors refer to legend in Fig. 6. Axes have been zoomed in to better highlight agreement between the Lagrangian-based fluxes and the corrected Eulerian fluxes.

436 vection velocity causes the numerical simulations to become unstable at such
 437 high values of τ_p .

438 If one interprets the last two terms of Eq. 11 as a correction to the iner-
 439 tialless turbulent flux, then a corrected turbulent flux can be defined:

$$\langle c'w' \rangle_{corr} = \langle c'w' \rangle - \langle C \rangle \tau_p \frac{\partial \langle w'^2 \rangle}{\partial z} - \tau_p \left\langle c' \frac{Dw'}{Dt} \right\rangle \quad (12)$$

440 which should approach the Lagrangian-computed turbulent flux for the iner-
 441 tial particles presented in Fig. 5. Figure 7 shows that this is indeed the case,
 442 however beginning at $St \approx 0.3$ the linear correction begins to break down. In
 443 this figure, the turbulent flux $\langle c'w' \rangle$ (“uncorrected” in Fig. 7) far overpredicts
 444 the vertical turbulent flux over much of the domain when v_j is modified to
 445 include the inertia. When adding the additional flux terms of Eq. 11 to $\langle c'w' \rangle$
 446 (“corrected” in Fig 7), the vertical turbulent flux nearly exactly matches the
 447 true flux predicted from the Lagrangian particles. While the corrected Eu-
 448 lerian flux diverges from the Lagrangian beginning at $St \approx 0.3$, the flux is
 449 fairly accurate through $St = 0.5$, suggesting that the key inertial effects on
 450 vertical fluxes have been captured by the linear correction to v_j . The resulting
 451 predictions of the vertical concentration profiles are likewise accurate up to
 452 $St \approx 0.3$, as shown in Fig. 8. The degree of success of inertial correction to v_j

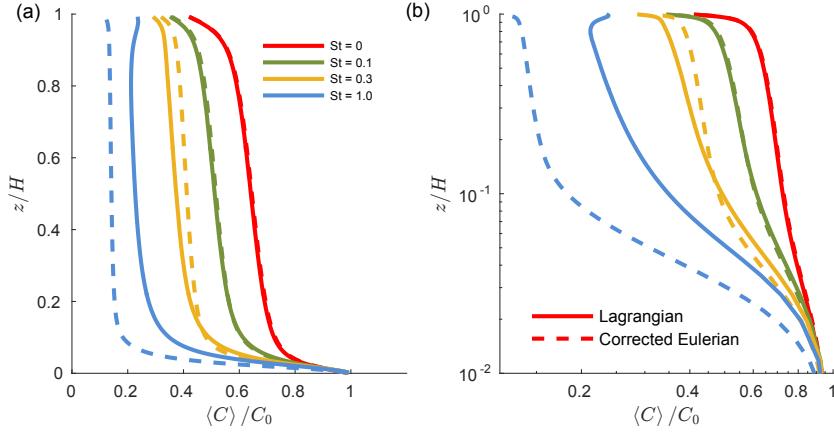


Fig. 8 Concentration profiles as predicted by the Lagrangian particles (solid lines) and the corrected Eulerian field (dashed lines). (a) Linear axes, (b) Logarithmic axes.

453 is in complete agreement with previous uses of the Equilibrium Eulerian model
 454 (Ferry and Balachandar, 2001).

455 3.4 Revisiting the Prandtl theory

456 The Prandtl solution for concentration (Eq. 9) was derived assuming a balance
 457 between turbulent suspension and gravitational settling. Furthermore, it uses
 458 a parabolic form of the eddy diffusivity, i.e., $K_C = \kappa u_* z (1 - z/H)$, which
 459 is the eddy diffusivity predicted by MO similarity theory in the presence of a
 460 linear momentum flux. As a first step, therefore, we compute K_C in the case of
 461 inertial particles to see how well a parabolic function compares with the eddy
 462 diffusivity implied by the ratio of the turbulent flux to the mean concentration
 463 gradient. For the corrected Eulerian flux this follows:

$$464 K_{C,E} = -\frac{\langle c' w' \rangle_{corr}}{\frac{\partial \langle C \rangle}{\partial z}}, \quad (13)$$

465 while for the Lagrangian-computed turbulent flux K_C is computed as:

$$466 K_{C,L} = -\frac{(\langle w_p \rangle + w_s) \langle C \rangle}{\frac{\partial \langle C \rangle}{\partial z}}, \quad (14)$$

467 where the numerator is the turbulent flux measured from the Lagrangian par-
 468 ticles, and inherently includes all true inertial effects.

469 Figure 9 shows both $K_{C,E}$ and $K_{C,L}$, and compares them to the parabolic
 470 solution assumed by MO theory. It is clear that the inertialess case ($St = 0$, red
 471 lines) follows the parabolic solution fairly closely, which is expected since the
 472 Prandtl solution was successful at predicting the mean concentration profiles

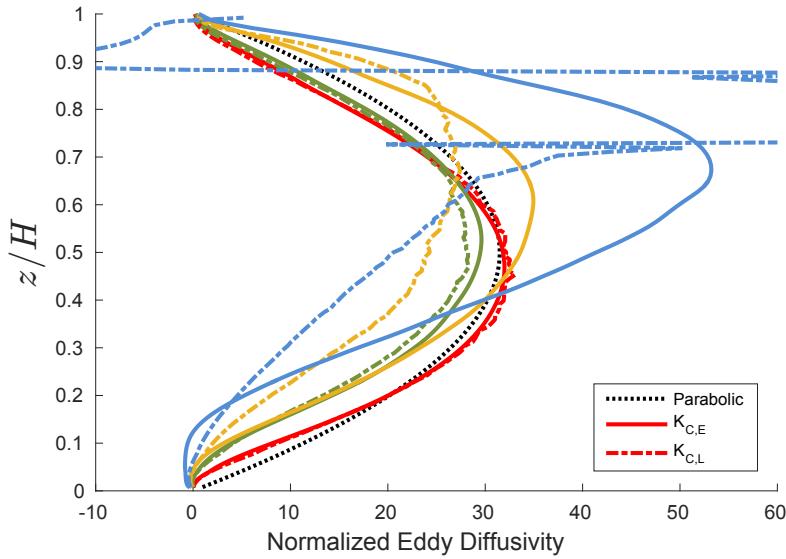


Fig. 9 Eddy diffusivities normalized by the molecular diffusivity Γ_C . Dotted black line represents the parabolic solution $K_C = \kappa u_* z (1 - z/H)$. Solid lines represent $K_{C,E}$ and dash-dotted lines represent $K_{C,L}$. Both profiles have been smoothed with an averaging filter. Colors follow legend of Fig. 8.

in Fig. 4. As St increases, however, not only do the computed eddy diffusivities deviate from the parabolic approximation, the Eulerian and Lagrangian predictions deviate from one another. Again, this is expected given the deviation between the corrected Eulerian and Lagrangian profiles shown in Fig. 7 and Fig. 8, since the Eulerian correction is only valid at low St . We note that the difference between $K_{C,L}$ and the parabolic solution is not simply a result of the so-called crossing trajectories effect: the correction proposed by Csanady (1963) for the vertical eddy diffusivity results in a vertical dispersion coefficient that is less than 1% different than the parabolic solution.

While the shape of both $K_{C,E}$ and $K_{C,L}$ is still somewhat parabolic at $St = 0.3$ (yellow lines in Fig. 9), the emergence of an inflection point in the concentration profile at $St = 1.0$ (see Fig. 8) causes $K_{C,L}$ to spike to very large and even negative numbers near $z/H \approx 0.8$. This behavior indicates that inertial particles violate the basic flux-gradient relationship assumed when defining an eddy diffusivity K_C , although the inertial correction to the Eulerian advection velocity compensates for this up to $St \approx 0.2$, as noted earlier.

It is instructive therefore to repeat the Prandtl analysis and attempt to predict the concentration profile while incorporating the inertial corrections to the Eulerian concentration field. The goal here is to determine whether or not a parabolic eddy diffusivity can be utilized for the uncorrected turbulent flux $\langle c'w' \rangle$ while capturing the inertial effects separately and explicitly. If this fails (which it indeed does), it would indicate that inertial effects must be

493 accounted for in the eddy diffusivity itself and not as a series of correction
 494 terms to the overall flux balance. If Eq. 11 is written as:

$$\langle c'w' \rangle - \langle C \rangle w_s + \beta(z) = 0, \quad (15)$$

495 where $\beta(z)$ represents the inertial corrections to the turbulent flux,

$$\beta(z) = -\langle C \rangle \tau_p \frac{\partial \langle w'^2 \rangle}{\partial z} - \tau_p \left\langle c' \frac{Dw'}{Dt} \right\rangle, \quad (16)$$

496 the analog to Eq. 8 assuming the parabolic form of the eddy diffusivity K_C is:

$$\kappa u_* z (1 - z/H) \frac{d \langle C \rangle}{dz} + \langle C \rangle w_s = \beta(z). \quad (17)$$

497 The solution to this inhomogeneous equation takes the following form:

$$\begin{aligned} \frac{\langle C \rangle(z)}{C_r} &= \left(\frac{z}{z_r} \right)^{-w_s/\kappa u_*} \left(\frac{z - H}{z_r - H} \right)^{w_s/\kappa u_*} \\ &+ \left(\frac{z}{H - z} \right)^{-w_s/\kappa u_*} \int_{z_r}^z \left(\frac{z}{H - z} \right)^{w_s/\kappa u_*} \frac{\beta(z)}{C_r \kappa u_* z (1 - z/H)} dz. \end{aligned} \quad (18)$$

498 Equation 18 contains the original Prandtl solution of Eq. 9 as the first term,
 499 followed by a correction which involves an integral of the inertial correction
 500 term $\beta(z)$. Since we do not have a closure for this term, we must integrate
 501 this term numerically, and its solution is presented in Fig. 10. Note that since
 502 $\langle C \rangle$ appears in the definition of $\beta(z)$, the numerical solution must be iterative;
 503 since the term containing $\langle C \rangle$ is small above $z_r = 0.3$ (Fig. 6(a)), however, the
 504 solution converges very rapidly.

505 Figure 10 shows that the correction indicated by Eq. 18 does not adequately
 506 modify the original Prandtl solution to account for inertia. This is of course
 507 true at the highest values of St (since again the inertial correction only is valid
 508 at low St), but even at $St = 0.3$ the additional term in Eq. 18 overcorrects
 509 the Prandtl solution substantially.

510 The reason behind this discrepancy is that the similarity-based, parabolic
 511 form of the eddy diffusivity K_C is no longer valid as St increases. If Eq. 8 is
 512 written using the Lagrangian-based $K_{C,L}$ as:

$$-K_{C,L} \frac{d \langle C \rangle}{dz} - \langle C \rangle w_s = 0, \quad (19)$$

513 then the solution for $\langle C \rangle$ can be computed numerically using the $K_{C,L}$ profiles
 514 presented in Fig. 9 (i.e. the dash-dotted lines). Note that Eq. 19 does not
 515 contain the inertial correction term $\beta(z)$ since the Lagrangian-based $K_{C,L}$
 516 inherently includes all inertial effects. Figure 10 shows that when solving Eq.
 517 19, the predicted concentration profile very closely matches the Lagrangian-
 518 based concentration profiles, except for regions near the inflection points in
 519 $\langle C \rangle$ where $K_{C,L}$ is ill-defined. Thus, the effects of particle inertia on vertical
 520 dispersion must not be limited to corrections to the turbulent flux (e.g. using

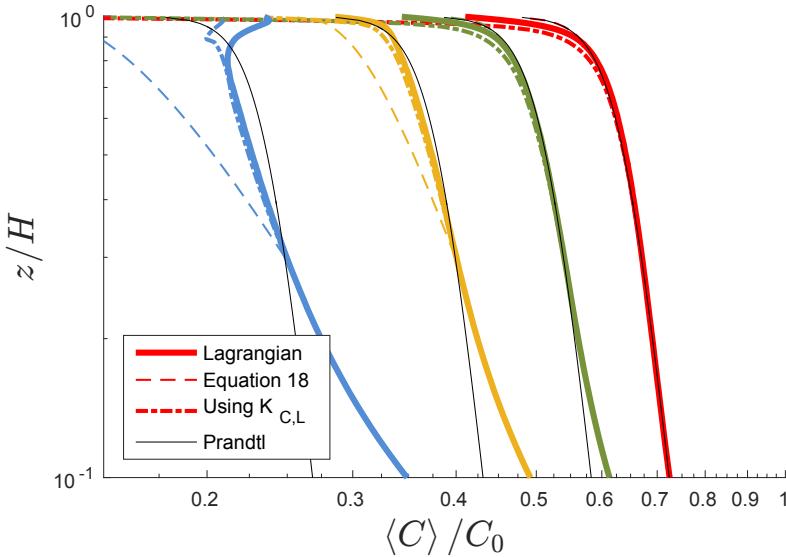


Fig. 10 Vertical concentration profiles computed from the inertial Lagrangian particles (solid lines) compared to the prediction of Eq. 18 (dashed lines). As before, $z_r = 0.3H$ and C_r is the concentration at this height, so the solution to Eq. 18 only exists above $z/H = 0.3$. Dash-dotted lines are the numerical solutions to Eq. 19, which uses the Lagrangian-based $K_{C,L}$, illustrating that the parabolic K_C becomes insufficient at high St . Colors refer to the legend in Fig. 8.

521 the Equilibrium Eulerian model to correct the particle advection velocity),
 522 but must also consider the fact that the eddy diffusivity, and therefore the
 523 relationship between the flux and the mean concentration gradient, is modified
 524 by inertia as well.

525 **3.5 Reynolds number**

526 Before demonstrating the effect of the inertial resistance layer in larger-scale
 527 models, we provide a comment upon the usage of direct numerical simulation,
 528 and thus the limitation in Reynolds number, of the current work. As the
 529 Reynolds number of this type of simulation increases towards the types of
 530 atmospheric flows we aim to investigate, the primary effect is to reduce the
 531 region over which molecular momentum and scalar diffusion dominate; indeed
 532 it is only outside of this region that the present work has focused. To this
 533 end, two additional simulations were run at a Reynolds number of $Re_\tau = 700$
 534 in order to demonstrate that the primary conclusions of this work remain
 535 intact. Figure 11 shows the counterparts to Figs. 4(b) and 9 for an inertialess
 536 and a $St = 0.1$ particle at the same dimensionless settling velocity. Figure
 537 11(a) shows that again, the inclusion of particle inertia causes a reduction in
 538 the concentration profile, and that the deviation from the Prandtl solution

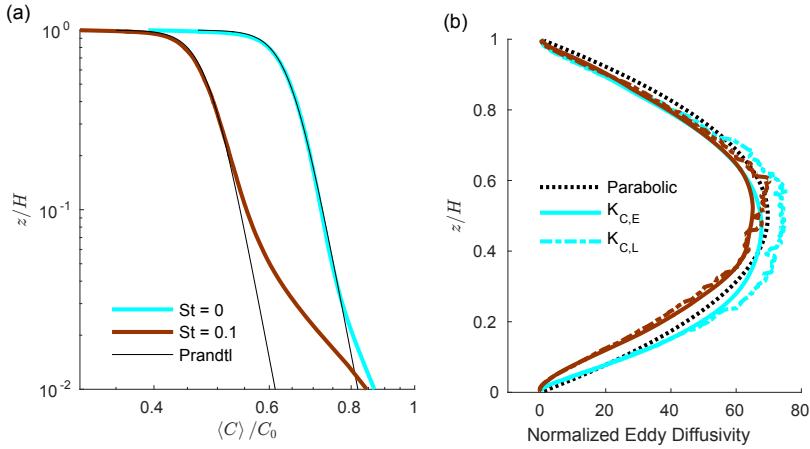


Fig. 11 (a) Concentration profiles and (b) eddy diffusivity profiles for $Re_\tau = 700$ cases for $St = 0$ (cyan) and $St = 0.1$ (dark red) particles. The trends are nearly identical to those presented in Figs. 4(b) and 9, respectively, illustrating the robustness of the present conclusions with increasing Re .

539 propagates from the lower wall upwards, beginning in regions with high local
 540 St . The only difference with the increased Reynolds number is that the range
 541 of agreement of the $St = 0$ case with the Prandtl solution extends further
 542 towards the lower surface, to $z/H \approx 0.02$ as opposed to $z/H \approx 0.08$ as before.
 543 The same is true in Fig. 11(b): the presence of inertia begins to alter the eddy
 544 diffusivity profile in a similar way to that of the lower Re cases, only in this
 545 case the magnitude of K_C is larger (as expected). Thus we argue that the
 546 methodology of using DNS as a tool for studying inertial particle fluxes in the
 547 lowest regions of the atmospheric surface layer is justified in that the effects
 548 of Reynolds number do not appreciably alter our basic findings.

549 3.6 Consequence of the inertial resistance layer

550 We argue above that within the first few meters above the emission layer, par-
 551 ticles often experience inertial effects as they are carried upwards by turbulent
 552 motions. In the DNS this is manifested as a reduction of the concentration
 553 profile at steady state, but can also be described as a reduction in the vertical
 554 turbulent flux above a particle source, similar to classic descriptions of depo-
 555 sition velocity resistance via molecular diffusion or vegetation canopies (Slinn
 556 and Slinn, 1980). In practice, this reduction in turbulent flux near the surface
 557 effectively reduces the emission flux felt by the boundary layer as compared
 558 to the true source flux. In this study we use DNS to resolve these near-wall
 559 motions to study their effect, but in practice these motions cannot be resolved
 560 and thus their effect must be parameterized.

561 To demonstrate this process, we perform a representative large eddy simu-
 562 lation (LES) using the unstable convective PBL studied in Freire et al. (2016).

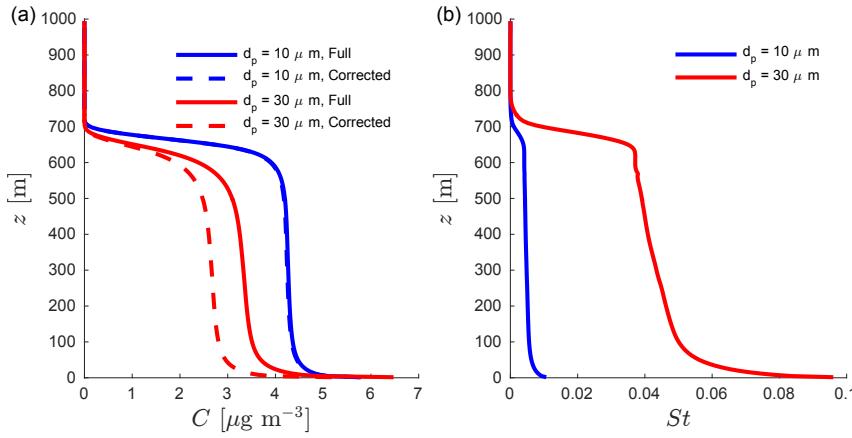


Fig. 12 (a) Concentration profiles of $d_p = 10 \mu\text{m}$ (blue) and $d_p = 30 \mu\text{m}$ (red) particles for the unstable convective PBL of Freire et al. (2016). Solid curves represent full surface fluxes of $0.2 \mu\text{g m}^{-2}\text{s}^{-1}$ and dashed lines represent surface fluxes corrected for inertial transport between the first grid point and the emission layer. (b) Stokes numbers of $d_p = 10 \mu\text{m}$ and $d_p = 30 \mu\text{m}$ particles, as computed by the subgrid dissipation of the LES scheme. From the perspective of LES, these particles are nearly inertialess, but can have significant inertial effects near the surface.

563 For an initial boundary layer height of $z_i = 570 \text{ m}$, a surface heat flux of
 564 0.24 K m s^{-1} , and a geostrophic wind of $U_g = 10 \text{ m s}^{-1}$, Eulerian concentration
 565 fields of $d_p = 10 \mu\text{m}$ and $d_p = 30 \mu\text{m}$ particles are solved, only taking into
 566 account gravitational settling and not explicitly accounting for inertia.

567 In Fig. 12(a), the solid curves represent the concentration profiles averaged
 568 between hours 3 and 4 for the same surface emission flux of $0.2 \mu\text{g m}^{-2} \text{s}^{-1}$.
 569 As expected, the heavier particles have lower concentrations throughout the
 570 PBL. To account for inertial effects at and beneath the first LES grid point,
 571 we estimate a surface Stokes number based on LES dissipation at the first grid
 572 point, and use Fig. 7 to provide a corresponding reduction in the surface flux
 573 due to the inertial resistance layer. For the case of $d_p = 10 \mu\text{m}$ particles, the
 574 local Stokes number at the bottom grid point is $St \approx 0.01$ and the corrected
 575 flux is estimated to be 99% of the original surface flux; the dashed blue line
 576 in Fig. 12(a) reflects this small difference. For the case of $d_p = 30 \mu\text{m}$ (dashed
 577 red line), however, the surface Stokes number is $St \approx 0.1$ and the reduction in
 578 surface flux is roughly 22%. Figure 12(a) highlights the fact that, as a result of
 579 this near-surface reduction of turbulent flux, mean concentrations throughout
 580 the entire PBL can be influenced by inertia near the surface. Furthermore,
 581 Fig. 12(b) shows that while inertial effects can lead to substantial changes in
 582 the predicted large-scale concentrations, particles in these regions do indeed
 583 appear nearly inertialess at these scales, as computed by their local Stokes
 584 number. Only near the surface do they begin to experience inertial effects, even
 585 possibly throughout the surface layer (see for example Nemes et al. (2017)).
 586 We again emphasize that the region of interest in this study, as simulated by

587 DNS, is within several meters of the surface (Fig. 3). By definition, LES in
 588 general cannot resolve the observed inertial behavior of the particles because
 589 it is a processes which occurs at the smallest scales of the turbulent flow.

590 4 Conclusions

591 In this work we seek to better understand the influence of particle inertia
 592 on vertical concentration profiles, and in particular the shortcomings of tra-
 593 ditional relationships that work well in low- or zero-inertia conditions (e.g.
 594 Prandtl (1952)). We utilize direct numerical simulations and Lagrangian point
 595 particles in turbulent open channel flow to explore the ability of inertial correc-
 596 tions to the Eulerian transport equation (i.e. the Equilibrium Eulerian model
 597 (Ferry and Balachandar, 2001)) to capture changes in the turbulent fluxes
 598 and concentration profiles. This numerical setup is meant to provide insight
 599 into the lowest $O(1\text{m})$ portion of the atmospheric surface layer, where wa-
 600 ter droplets or sand/dust grains will experience inertial influences on their
 601 trajectories between the time they are emitted and the subsequent transport
 602 throughout the whole PBL.

603 We find that while the primary balance governing the concentration of
 604 suspended particles remains between turbulent flux and gravitational settling,
 605 both fluxes are reduced in magnitude and cause a reduction of particle con-
 606 centration at a specific height. This reduction in concentration increases with
 607 particle Stokes number, and reflects an inability of the particle to be instan-
 608 taneously transported with the local fluid motion. Up to a Stokes number
 609 of approximately $St \approx 0.3$, the Equilibrium Eulerian framework provides a
 610 viable means for correcting the turbulent flux, and thus can reproduce iner-
 611 tial particle profiles accurately. Above this threshold, however, this first-order
 612 correction fails to reproduce behavior seen by the Lagrangian particles. In
 613 all cases, as the Stokes number is increased, the turbulent flux becomes less
 614 well represented by a similarity-based eddy diffusivity, and any attempt at
 615 parameterizing the vertical turbulent flux must begin with a more accurate
 616 description of the effective, inertia-influenced eddy diffusivity.

617 The result is that atmospheric weather prediction or large eddy simulation
 618 models, which attempt to predict the transport of spray, dust, snow, etc.,
 619 may overestimate airborne concentrations if an inertialess, similarity-based
 620 theory is used to link traditional emission schemes (e.g., saltation models,
 621 sea spray generation functions) to the flux at the first grid point above the
 622 lower surface. Likewise in practice, surface emission parameterizations may
 623 underestimate true emission if airborne concentration observations are used
 624 to infer surface fluxes. Since particles must traverse through the first several
 625 meters of the surface layer before arriving at elevations corresponding to the
 626 first grid point in numerical models, they have necessarily experienced some
 627 inertial transport along the way. The present results suggest that this inertial
 628 behavior may result in a decrease in vertical fluxes compared to traditional
 629 predictions.

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