Direct numerical simulations of particle transport in a model estuary

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We investigate numerically the mixing of freshwater with ambient saltwater in a model estuary along with associated particle settling processes. We first discuss and specify two numerical setups that consider several relevant features to study the particle settling. The first configuration is a large rectangular basin with a small inlet for the (particle-laden) freshwater; the second is geometrically identical to the first except that the flow is laterally confined to the narrow inlet width. The two flows are computed until a statistically stationary solution is reached. We perform highly resolved direct numerical simulations using a high-order finite difference approach to yield reliable and accurate results. Accordingly, all relevant turbulent scales are resolved and turbulence modeling is not needed. The main target of this study is to describe and illustrate the fluid dynamics and the particle settling processes under the influence of turbulence arising in the freshwater/saltwater-stratified mixing layer. To this end we analyze and compare the two simulations with respect to different aspects of the freshwater/saltwater interaction and to the transport and settling processes of the particles. We investigate the spatial structure as well as the temporal evolution of the flows and the particle suspensions. Generally, we find a qualitatively good agreement of both numerical simulations with pertinent laboratory experiments. Particularly, the results confirm a significant enhancement of the particle settling speeds compared to pure Stokes settling in the presence of turbulence. However, we also demonstrate that the results for the two configurations differ fundamentally in several aspects: stability of the freshwater/saltwater interface, degree of turbulent mixing, particle plume expansion and particle settling enhancement. Using these two simulations we explain the observed settling enhancement, which is not related to the particle inertia (as it is not considered in the numerical model) but rather to the buoyancy velocity of the particle suspension and the geometry of the estuary mouth configuration.

Keywords: estuary mouths; turbulent mixing; sedimentation; particle settling; particle deposition; numerical simulation; feedback-coupled particles; flume experiments

1. Introduction

The details of freshwater mixing with ambient brine in estuaries as well as the transport of suspended particles to the ocean are not fully understood [1–6]. The transport mechanisms of natural sediment and pollutants are especially of interest because up to 10 billion metric tons of sediment are transported annually by rivers to continental shelves [7], which is of great importance for the marine environment.

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In most cases, the freshwater–particle mixture is lighter than the saltwater near the estuaries, such that the river plumes are positively buoyant. Thus, the particles can be transported over relatively large distances with the freshwater current. The expansion of the particle plume is only limited by the particle settling that dominates over the horizontal transport with growing distance to the river mouth. However, the settling mode is somewhat controversial in the literature; the only agreement is that Stokes settling of disaggregated constituent grains cannot account for the sediment flux out of typical rivers [4, 5]. The traditional assumption for an enhanced particle settling is the flocculation of individual particles because larger effective aggregate diameters lead to larger Stokes settling speeds [3, 8]. More recent studies favor the positive influence of turbulence on the effective particle settling velocity [4, 6]. In genuine estuaries turbulence is mostly generated by the kinetic energy of the freshwater inflow, wind stresses, tides and/or other ambient seawater currents. Even the potential energy of the particle suspension in the buoyant freshwater current may contribute to an enhanced settling mechanism.

The main objective of the present study is an accurate description of the freshwater/saltwater mixing, the particle transport and, most of all, the (enhanced) particle settling in a model estuary. The enhancement of particle settling due to turbulence has been demonstrated in different (rather idealized) laboratory experiments and numerical simulations for homogeneous isotropic turbulence (e.g. [9–11]). Pertinent laboratory experiments for the particle settling under estuary conditions, for instance, have been conducted by Maxworthy [12], Parsons et al. [6] and McCool and Parsons [4]. These studies were restricted by a couple of practical limitations that we can overcome by our numerical simulation setups. However, our designs still orient themselves on these experiments, especially on [4], such that qualitative comparisons between the results are feasible.

Numerical simulations of estuary mouths are well established in geophysical research (e.g. [13–22]). These studies typically focus on real-life examples and try to consider almost all physically relevant effects. Besides the sediment transport, Coriolis forces, tidal currents, wind-induced stresses and other ambient alongshore currents are also often considered. Because of the large scale of natural rivers it is impractical nowadays to fully resolve these flows and to simulate them by means of Direct Numerical Simulation (DNS). Instead, Large-Eddy Simulation (LES) is employed in combination with eddy-diffusion models, which are, in most cases, related to the Smagorinsky closure [23]. The advantages of LES over the numerical simulation of the Reynolds-Averaged Navier–Stokes equations have been discussed by Roman et. al. [22] for coastal flows. As far as possible, most of the aforementioned studies also try to resolve the coastlines and bathymetries of specific estuaries. Typically, boundary-fitted meshes are employed for this purpose and also the Immersed Boundary Method has been applied successfully [22]. However, there are also attempts to use more abstract model configurations to study basic effects (e.g. [20, 19]). Many of these works employ standardized simulation codes, such as the Princeton Ocean Model [24]. However, even for laboratory-scale problems these numerical studies are limited to strongly simplified configurations and/or have to introduce relatively strong model assumptions. These restrictions are – to a large extent – attributable to limited computing resources and/or to the scalability of the numerical models.

We present an appropriate numerical model that allows high-resolution simulations of estuary mouth flows. We solve the flow by means of DNS for which modeling is reduced to a minimum. The advantage of this approach is that all relevant length and time scales, ranging from small interface thicknesses or turbulence eddies to the large Kelvin–Helmholtz-type (K–H) vortical flow structures, can be represented accurately. As has been stated before, genuine river flows are out of reach of DNS and we can focus only on laboratory-scale
problems because the numerical effort grows rapidly with the resolution requirements. However, with today’s computing power we are able to conduct nearly realistic numerical simulations. The laboratory-scale flows still reveal a large range of different scales that allows us to study the fundamental mechanisms at a high level of accuracy. We employ a newly developed simulation code for the incompressible Navier–Stokes equations that is based on high-order finite differences and runs very efficiently on today’s large massively parallel supercomputers [25, 26].

As has been stated above we are particularly interested in the particle transport and the basic particle settling mechanism. Generally, there are different influences acting on the particle motion, from which we try to comprise only the most relevant ones in our setup. More precisely, we consider as most important the buoyancy forces arising from the salinity and the particle suspension, the momentum of the freshwater–particle inflow and the turbulent mixing of all phases. Correspondingly, all other effects are neglected, i.e. Coriolis forces due to earth rotation, tidal currents, wind-induced stresses, temperature gradients and ambient alongshore currents. Normally, these influences are also not considered in typical laboratory-scale experiments, cf. e.g. [4, 6, 12]. As no flocculation was observed in any of these studies, we will not take this feature into account either. Furthermore, we neglect the inertia of individual particles from which we expect only a minor influence in this context, as explained later. However, it should be mentioned that particle inertia is an essential model feature for the settling enhancement in homogeneous isotropic turbulence (e.g. [9–11]).

To this end we first introduce two geometrically different estuary configurations for laboratory-scale flows, specify the relevant characteristic numbers and discuss typical values for these parameters (Section 2). In Section 3 we discuss the governing equations, followed by the specification of appropriate boundary and initial conditions in Section 4. The discretization and the numerical solution procedure are briefly described in Section 5. The physical results are presented in Section 6 (freshwater/saltwater interaction) and Section 7 (particle transport and settling). Finally, the assumptions made in our particle model are briefly verified a posteriori (Section 8) and the results summarized in Section 9.

2. Configuration and characteristic numbers

To study the freshwater/saltwater mixing as well as the particle transport in a model estuary we consider two different types of configurations that are depicted in Figure 1: The first is a large open basin (OB) with a relatively small inlet for the freshwater (and suspended particles at later times); and the second is identical to the first except that the flow is laterally confined to the width of the inlet resembling a confined channel (CC). Obviously, the first configuration is geometrically closer to a real estuary, whereas the second is often used in laboratory experiments, e.g. [4]. Both basins are rectangular boxes with extents \( \tilde{L}_1 \times \tilde{L}_2 \times \tilde{L}_3 \) (a tilde \((\tilde{\cdot})\) denotes dimensional quantities) that are discretized on Cartesian grids with coordinates \( \tilde{x}_1, \tilde{x}_2, \tilde{x}_3 \). The inflow boundary plane, \( \tilde{x}_1 = 0 \), is specified as ‘I’, the outflow boundary planes as ‘O’, the top of the basin as ‘T’ and the bottom as ‘B’.

In our parameter range, cf. Section 2.3, the pure freshwater as well as the particle-laden freshwater are lighter than the ambient saltwater. Therefore, the saltwater is typically located in the lower part of the domain and it is suggestive to establish the inlet directly below the water surface. The inlet depth is denoted as \( \tilde{h} \), the inflow bulk velocity as \( \tilde{U} \) and the gravitational acceleration, \( \tilde{g} \), acts in the negative \( \tilde{x}_3 \) direction, \( e^g = \{0, 0, -1\}^T \), cf. Figure 1. The width of the inlet and the total basin depth is \( 4\tilde{h} \), such that the relations
between inlet depth, channel width and depth coincide approximately with McCool and Parsons [4] laboratory configurations.

To save computational effort, we introduce a symmetry plane at \( \tilde{x}_2 = 0 \) in both configurations that does not seem to have an important effect on the flow. The confinement in the second configuration is established by a symmetry plane at \( \tilde{x}_2 = 4h \). To ensure that we always have a sufficiently large amount of salinity inside the basin, we additionally establish a fringe region [27] for the salinity at the outflow (cf. also Section 4).

Besides \( \tilde{U}, \tilde{h} \) and \( \tilde{g} \), we use the kinematic viscosity \( \tilde{\nu} \), the freshwater density \( \tilde{\rho}_f \), the maximum saltwater density \( \tilde{\rho}_{\text{sal}} \), the particle density \( \tilde{\rho}_{\text{part}} \), the particle diameter \( \tilde{d} \), the maximum particle volume fraction of the particle suspension, \( \tilde{\phi}_V \), the diffusivities \( \tilde{D}_{\text{part}} \) and \( \tilde{D}_{\text{sal}} \) of the particle suspension and the salinity as the reference quantities for our simulations. With the reduced gravitational accelerations,

\[
\tilde{g}_{\text{part}} = \frac{\tilde{\rho}_{\text{part}} - \tilde{\rho}}{\tilde{\rho}} \tilde{g} \tilde{\phi}_V, \quad \tilde{g}_{\text{sal}} = \frac{\tilde{\rho}_{\text{sal}} - \tilde{\rho}}{\tilde{\rho}} \tilde{g},
\]

(1)
we define the dimensionless characteristic numbers

\[ Re \equiv \frac{\tilde{U} \tilde{h}}{\tilde{v}}, \quad Ri_k \equiv \frac{\tilde{g}^k \tilde{h}}{\tilde{U}^2}, \quad Sc_k \equiv \frac{\tilde{v}}{D_k}, \]  

(2)

where the index \( k \) may be either ‘part’ or ‘sal’. \( Re \) denotes the Reynolds number, \( Ri_k \) the Richardson numbers and \( Sc_k \) the Schmidt numbers. Further, the particles are characterized by the Stokes number \( St \) and the nondimensional particle Stokes settling velocity \( u_{part}^s \) (acting in gravity direction \( e^g \)),

\[ St \equiv \frac{\tilde{d}^2 \tilde{\rho}_{part} \tilde{U}}{18 \tilde{v} \tilde{\rho} \tilde{h}}, \quad u_{part}^s \equiv e^g \frac{\tilde{\rho}_{part} - \tilde{\rho}}{\tilde{\rho}} \frac{\tilde{d}^2 \tilde{g}}{18 \tilde{v} \tilde{U}}. \]  

(3)

As we wish to have at least a qualitative agreement with the experiments of McCool and Parsons [4], we try to comply with their physical parameters as far as possible. Their characteristic numbers are not explicitly given but we can estimate them from the context. To compare our results with these experiments, we assume the same gravitational acceleration, viscosities and densities of freshwater, saltwater and suspended particles. The parameter ranges for the experiments are listed in Table 1 along with our choices. We will discuss these below in detail. Other pertinent laboratory experiments were conducted by Maxworthy [12] and Parsons et al. [6]; however, these studies employ configurations that differ more from ours than [4] such that we will consider them only if expedient.

### 2.1. Stokes number and Stokes settling velocity

Generally, we try to choose the horizontal extents \( \tilde{L}_1 \) and \( \tilde{L}_2 \) of the domain sufficiently large to avoid the particles leaving the domain via the outflow ‘O’ and thus allowing almost all of them to deposit on the ground. We know from numerical experiments that the horizontal expansion of the particle plume is mostly governed by the magnitude of the Stokes settling
Table 2. Spatial extents and grid resolutions of two numerical configurations for the model estuary, cf. Figure 1.

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>$L_1 \times L_2 \times L_3$</th>
<th>$N_1 \times N_2 \times N_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Open basin OB</td>
<td>$80 \times 50 \times 4$</td>
<td>$2305 \times 1153 \times 193$</td>
</tr>
<tr>
<td>Confined channel CC</td>
<td>$80 \times 4 \times 4$</td>
<td>$3073 \times 193 \times 193$</td>
</tr>
</tbody>
</table>

velocity $\bar{u}_{\text{part}}$. As the computational expense grows with the domain length and width, we employ slightly larger particles than in the experiments [4] to obtain a faster settling speed according to Stokes’ law, i.e. Equation (3). Ultimately, the nondimensional particle settling speed is set to $|\bar{u}_{\text{part}}| = 0.02$ and the spatial extents of the first computational domain are chosen as $L_1 \times L_2 \times L_3 = 80 \times 50 \times 4$ and of the second as $80 \times 4 \times 4$, cf. Table 2.

The relation between the particle Stokes settling velocity and the particle Stokes number can be computed from Equation (3),

$$\frac{|\bar{u}_{\text{part}}|}{St} = \left[ 1 - \frac{\tilde{\rho}}{\tilde{\rho}_{\text{part}}} \right] \tilde{g} \tilde{h} \tilde{U}^2.$$  

(4)

Obviously, $|\bar{u}_{\text{part}}|/St$ is (for given $\tilde{\rho}, \tilde{\rho}_{\text{part}}$, cf. Table 1) only a function of $\tilde{h}$ and $\tilde{U}$ but not of the particle diameter $\tilde{d}$. As we choose $\tilde{h}$ and $\tilde{U}$ to match the other characteristic numbers, our particle Stokes number is also slightly larger than that of the experiments.

2.2. Reynolds and Schmidt numbers

The resolution quality of a DNS can be assessed using the so-called grid Péclet number [28],

$$P_{\text{Pe}, \Delta} \equiv \max_{x,i} \{ \mu u_i \Delta x_i \}, \quad i = 1, 2, 3, \quad \mu \equiv Re \max \{ 1, Sc_{\text{part}}, Sc_{\text{sal}} \}.$$  

(5)

The lower the $P_{\text{Pe}, \Delta}$, the better the quality of the numerical solution. From previous numerical experiments (e.g. [29, 30]) we know that our discretization predicts even the smallest flow features reasonably accurately if the grid Péclet number, $P_{\text{Pe}, \Delta}$, is roughly below 100.

The Reynolds numbers in the laboratory experiments of McCool and Parsons [4] were on the order of 5000 to 10,000, which is generally within reach for a time-dependent and accurate numerical simulation of the desired flow problem, e.g. by means of LES or even DNS. The Schmidt number $Sc_{\text{sal}}$ of the salinity, however, is typically on the order of hundreds to thousands and the Schmidt numbers $Sc_{\text{part}}$ of particle suspensions are of even much higher order. Such values are currently not feasible in our DNS and are to be reduced because we want to maintain grid Péclet numbers within the order of 50 to 100. On the other hand, recent numerical studies of density-driven currents indicate that the structure and dynamics of such flows depend only weakly on the Schmidt number if the Reynolds number is sufficiently large and the Schmidt number not much lower than unity [31, 32]. Although our flow configuration is not only density-driven, we can assume that these findings also apply for our simulations.

Ultimately, we reduce the Schmidt numbers to $Sc_{\text{sal}} = 1$ and $Sc_{\text{part}} = 2$ to avoid very fine grids resolving steep gradients for $Sc_{k} \gg 1$ and thus substantial increases of computational cost. The difference in the Schmidt numbers is chosen to account at least for the difference
between the diffusivities of the particle suspension and the salinity, e.g. required for double-diffusive sedimentation (cf. e.g. [6]). The reduction of the Schmidt numbers allows us to increase the Reynolds number to $Re = 1500$, which is large enough to admit turbulence and to render the basic particle settling effects, although it is still smaller than the numbers of the experiments [4]. We resolve the first configuration spatially with $N_1 \times N_2 \times N_3 = 2305 \times 1153 \times 193$ grid points together with a moderate grid stretching in the horizontal directions and the second configuration with $3073 \times 193 \times 193$ grid points without any grid stretching (cf. Figure 1 and Table 2).

2.3. Richardson numbers

The Richardson number relates the potential energy due to density differences to the kinetic energy of a flow. The relative density difference $(\bar{\rho}_{\text{sal}} - \bar{\rho})/\bar{\rho}$ between freshwater and saltwater was fixed to 0.015 in all the experiments conducted by Parsons et al. [6], whereas the contribution of the suspended particles to the overall density was smaller at least by a factor of two. These numbers refer to ‘typical’ values of genuine estuaries [8, 33, 34]. Note that both density differences may vary strongly in nature: The average relative density difference between oceanic saltwater and freshwater is around 0.035 and for seawater it is in the range of 0.03 ... 0.038. Even these values can be exceeded by the particle suspension [5, 6, 35]. In the case where the freshwater/particle inflow is denser than the ambient fluid, the inflow becomes negatively buoyant (‘hyperpycnal’) in contrast to the present situation where the inflow is positively buoyant (‘hypopycnal’), for instance cf. [6].

The Richardson number of the inflow can be approximated by $Ri_{\text{inflow}} \approx Ri_{\text{sal}} - Ri_{\text{part}}$ for our configuration (cf. Section 4 and Figure 1). For hypopycnal inflows, $Ri_{\text{inflow}}$ is positive whereas it is negative for the hyperpycnal case. Further, the inflow is sub-critical for $Ri_{\text{inflow}} \lesssim 1$ and supercritical for $Ri_{\text{inflow}} \gtrsim 1$, which determines whether or not a hydraulic jump occurs behind the inflow and disturbances can move upstream. We consider a hydraulic jump as unphysical in our configuration because it would be retained artificially in the basin by the inflow boundary condition, whereas the saltwater in a real experiment would propagate upstream into the water supply. On the other hand, a strongly supercritical inflow occurs only if its kinetic energy is much larger than the potential energy corresponding to the density difference between fluid and displaced ambient fluid, e.g. for strongly inclined water supplies and/or small density differences.

As $Ri_{\text{inflow}} \gtrsim 1$ is obviously a free parameter, we set $Ri_{\text{sal}} = 0.5$ and $Ri_{\text{part}} = 0.05$ in our simulations to obtain a slightly supercritical inflow. These choices agree well with the laboratory setup of McCool and Parsons [4] although our salinity Richardson number is rather at the lower end of their parameter range.

3. Governing equations

The motion of an individual particle in a fluid can be described accurately by the well-established Maxey–Riley equation of motion [36]. As typical riverine sediment mainly consists of small and heavy particles (cf. [4] and Table 1), we can employ a simplified form of this equation [37],

$$
St \frac{dv(t)}{dr} + v(t) = u_s(x(t), t) + u_{\text{part}},
$$

(6)
where \( v \) is the nondimensional particle velocity, \( u \) the fluid velocity and \( t \) the time. The nondimensional position \( x(t) \) of an individual particle is determined from the trajectory equation,

\[
\frac{dx(t)}{dt} = v(t).
\]  

(7)

If the fluid velocity \( u \) is known in advance, the analytic solution of Equation (6) is given by

\[
v(t) = u(x(t), t) + u_{\text{part}}^{s} + e^{-\frac{t-t_0}{\text{St}}} \left[ v(t_0) - \int_{t_0}^{t} e^{-\frac{\tau-t_0}{\text{St}}} \frac{du(x(\tau), \tau)}{d\tau} d\tau \right].
\]  

(8)

Generally, the initial condition \( v(t_0) \) is almost irrelevant for typical particle Stokes numbers (cf. [4] and Table 1). Further, we can assume that the particle suspension is only weakly feedback coupled to the fluid, as indicated by its small Richardson number. Hence, \( u(x(t), t) \) is only slightly influenced by the particle motion and we find that the last term on the right-hand side of Equation (8) is limited by

\[
e^{-\frac{t-t_0}{\text{St}}} \left| \int_{t_0}^{t} e^{-\frac{\tau-t_0}{\text{St}}} \frac{du(x(\tau), \tau)}{d\tau} d\tau \right| \lesssim 2\text{St}_{\text{max}} \left| \frac{\partial u(x, t)}{\partial t} \right| \equiv \text{St}A.
\]  

(9)

Note that this upper limit is strictly applicable only for one-way coupled particles with \( R_{\text{part}} \equiv 0 \). We will demonstrate a posteriori (cf. Section 8) that the upper bound \( \text{St}A \) is sufficiently small compared to \( |u_{\text{part}}^{s}| \) for the areas of interest so that Equation (6) can be well approximated by

\[
v(t) = u(t) + u_{\text{part}}^{s}.
\]  

(10)

As indicated by Equation (9), this approach is adequate for weak turbulent flows, see also Maxey et al. [38] for further details. The particle acceleration term in Equation (6) is known to contribute to an enhanced particle settling under the influence of turbulence, cf. e.g. [9–11]. Hence, the reduced model, Equation (10), may simplify the identification of other settling enhancing effects.

The equivalent Eulerian description of Equations (7) and (10) is given by

\[
\frac{\partial c_{\text{part}}}{\partial t} + (u + u_{\text{part}}^{s}) \cdot \nabla c_{\text{part}} = 0,
\]  

(11)

where the particles are represented by a volumetric particle concentration \( c_{\text{part}} \) (i.e. a differential number of particles per volume). Diffusive terms are already neglected in Equations (6), (7) and (10) due to the very low diffusivity of typical particle suspensions, which implies that Equation (11) will reveal very sharp interfaces of \( c_{\text{part}} \). As the discretization limits all interface thicknesses to the local grid spacing \( \Delta x \), independently on the point of view, we cannot represent the very low particle diffusivity on a typical mesh (see also the discussion in Section 2.2 on the Schmidt numbers). To this end, we introduce a diffusive term on the right-hand side of Equation (11) to have at least a direct control of the particle diffusion and to permit diffusivity differences between different concentrations. For salinity such a treatment is straightforward anyway (the concentration is denoted by \( c_{\text{sal}} \)) such that the corresponding nondimensional transport equations for each of the concentrations \( c_{\chi} \)
can be formulated as

\[
\frac{\partial c_k}{\partial t} + \left( (u + u^s_k) \cdot \nabla \right) c_k = \frac{1}{Re Sc_k} \Delta c_k, \quad k = \text{part, sal},
\]

with \( u^s_{\text{sal}} \equiv 0 \).

The density differences due to salinity and suspended particles lead to additional volumetric forces on the carrier fluid. As all density variations are very small compared to the mean density (cf. Section 2.3 and Table 1), we can apply the Boussinesq approximation at negligible error. As we consider only small spatial domains and short time spans in our simulations, we can also neglect the influence of Coriolis forces due to earth rotation that are of great importance for large-scale estuaries only (cf. [21]). With these assumptions the dimensionless incompressible Navier–Stokes equations read

\[
\frac{\partial u}{\partial t} + (u \cdot \nabla) u = -\nabla p + \frac{1}{Re} \Delta u + e^g \sum_k Ri_k c_k, \quad k = \text{part, sal},
\]

\[
\nabla \cdot u = 0,
\]

where \( p \) denotes the pressure (divided by the mean fluid density).

For Equations (12) and (13) we employ either Dirichlet boundary conditions,

\[
c_k = c^0_k, \quad u = u^0,
\]

or no-flux and advective boundary conditions, respectively,

\[
u^e_k c_k - \frac{1}{Re Sc_k} \frac{\partial c_k}{\partial e^n} = 0 \quad \text{for} \quad u^e_k \leq 0,
\]

\[
\frac{\partial c_k}{\partial t} + u^e_k \frac{\partial c_k}{\partial e^n} = 0 \quad \text{for} \quad u^e_k > 0,
\]

\[
\frac{\partial u}{\partial t} + U^n \cdot e^n \frac{\partial u}{\partial e^n} = 0 \quad \text{with} \quad U^n \cdot e^n \geq 0,
\]

where \( e^n \) is the unit outer normal vector, \( u^e_k \equiv (u + u^s_k) \cdot e^n \) is the advection velocity of the concentration \( k \) and \( U^n \) is the advection velocity of the fluid on the boundary (\( U^n \) must be specified, cf. Section 4). For instance, this set of boundary conditions was also used in [31]. The homogeneous Robin boundary condition (Equation 15a) prohibits an advective flux into the computational domain by enforcing an appropriate gradient \( \partial c_k / \partial e^n \leq 0 \) for \( c_k \geq 0 \) (and vice versa) on the boundary. Boundary conditions (15b) and (15c) are used to transport disturbances out of the domain. Note that Equation (15c) also permits velocities \( u \cdot e^n < 0 \), i.e. it can act as an inflow boundary condition. Therefore, the magnitude of \( U^n \cdot e^n \geq 0 \) must be sufficiently large to keep inflow velocities \( u \cdot e^n < 0 \) close to zero and also to avoid unphysical reflections for \( u \cdot e^n \geq 0 \). This prerequisite excludes the velocity \( u \) as a more “natural” choice for the advection velocity \( U^n \). Advective boundary conditions, such as Equations (15b) and (15c), were analyzed in detail in [39].
4. Boundary and initial conditions

We specify the inlet profile for the velocity and for the concentrations at ‘I’ as

\[ u^0 = (f, 0, 0)^T, \quad c_{\text{part}}^0 = f \quad \text{and} \quad c_{\text{sal}}^0 = 1 - f, \quad (16) \]

respectively (cf. Equation (14)). For the open basin the function \( f \) is given by

\[ f(x_2, x_3, t) = \frac{1}{4} \left[ 1 - \text{erf}\left( \frac{\sqrt{\pi } x_2}{\delta} \right) \right] \left[ 1 + \text{erf}\left( \frac{\sqrt{\pi } (x_3 - x_3^m(t))}{\delta} \right) \right], \quad (17) \]

and for the confined channel, \( f \) is defined as

\[ f(x_3, t) = \frac{1}{2} \left[ 1 + \text{erf}\left( \frac{\sqrt{\pi } (x_3 - x_3^m(t))}{\delta} \right) \right], \quad (18) \]

where \( \delta \) is the inflow shear layer thickness and \( x_3^m(t) \) is the vertical position of the interface.

As we want to study the effect of turbulence on the particle settling, we need to provide a large range of different turbulent length and time scales in the basin. To this end we choose a small shear layer thickness \( \delta \) at the inflow boundary to destabilize the stratified flow and to trigger large-scale disturbances, such as the Kelvin–Helmholtz or Holmboe waves (which may break down into turbulence farther downstream), in the freshwater/saltwater interface. Such disturbances are found in nature [40] and were also observed in the experiments of McCool and Parsons [4]. In either case, the shear layer thickness must still be resolved by the grid so that we set \( \delta = 0.1 \) as a compromise. From a linear stability analysis of the inflow profile at \( x_1 = x_2 = 0 \) we can confirm that it is unstable. Practically, however, the rather high salinity diffusion plays a significant role in this context because it spreads the interface profile downstream rapidly and diminishes the growth rates strongly. Hence, we excite the instability of the shear flow additionally by introducing small disturbances, or more specifically, by moving the vertical position of the interface \( x_3^m(t) = x_3^0 + x_3^\text{rand}(t) \) randomly around the average position \( x_3^0 = 3 \). The random contribution is derived for each grid line in the \( x_2 \)-direction separately from the so-called Ornstein–Uhlenbeck process [41] with relaxation time \( t_{\text{relax}} = 1000 \) and variance \( \text{var}[x_3^\text{rand}] = 0.005^2 \). Especially with small \( \delta \) our inflow configuration is obviously reminiscent of a flow over a backward-facing step, which, for instance, was employed in the experiments by McCool and Parsons [4].

Next, the outflow ‘O’ is modeled with boundary conditions (Equations (15)) and \( U^n = (1, 0, 0)^T \) at \( x_1 = L_1 \) and \( U^n = (0, 1, 0)^T \) at \( x_2 = L_2 \). As these boundary conditions would successively wash the salt concentration out of the domain, we replace Equation (15a) by \( c_{\text{sal}}^0 = 1 \) for \( n_{\text{sal}}^0 \leq 0 \) and additionally use a fringe region [27] for the salinity to ensure that an appropriate and unique statistically stationary state exists for late times (cf. Figure 1).

The motivation for this set of boundary conditions is the approximate hyperbolic character of the transport Equation (12) and the momentum Equation (13a) for large concentration and fluid scales, respectively, for which the diffusive terms are small compared to the advective terms. Because we choose relatively large streamwise extents for the two basins, smaller flow features have enough time to decay before they reach the outflow boundary. We experimentally checked that the flow in the area of interest is almost independent of the outflow parameter \( U^n \) (under the restrictions discussed in Section 3), which indicates that the advective boundary conditions are well suited to mimic ‘infinitely’ large basins.
Finally, the bottom ‘B’ is modeled as a no-slip boundary (i.e. $u^0 = 0$) and the top ‘T’ as a nondeformable free-slip (i.e. symmetry) boundary for the fluid. Accordingly, Equations (15a) and (15b) are used in the vertical direction to model appropriate boundary conditions for the concentrations. Practically, the advective boundary condition (Equation (15b)) on the ground, $x_3 = 0$, advects the particle concentration with the Stokes settling velocity out of the domain. From the physical point of view, however, we assume that the particles deposit on the ground and do not resuspend. The deposit height can be assumed to be negligible as the flow is computed only until $t = 1600$, cf. the parameter values given in Table 1.

The initial conditions for the velocity and the salt concentration in all $x_2$–$x_3$ planes along the $x_1$-coordinate are identical to the inflow boundary condition with $x_3^{\text{rand}}(0) = 0$. The influence of the salinity on the flow dominates over the effect of the particles due to the large difference between the corresponding Richardson numbers. We add the particles to the freshwater inflow beginning at $t = 250$. At this time the pure freshwater/saltwater interaction has attained a proper statistically steady state.

5. Numerical approach

Equations (12) and (13) with boundary conditions of Equation (14) and/or Equations (15) are discretized in space and time for a numerical solution. Centered, explicit and sixth-order accurate finite differences on staggered grids are chosen for the spatial discretization away from the boundaries. Only the advective terms are discretized with the fifth-order upwind-biased finite differences [42] because our grid will not be fine enough to fully suppress grid point oscillations (cf. the discussion on the grid Péclet number in Section 2.2). All differentiation and interpolation operations at the boundaries are at least fourth-order accurate.

In case the viscous time-step limit is more restrictive than the convective one, the diffusive terms are treated implicitly in time with the Crank–Nicolson scheme. Otherwise, the low-storage, third-order accurate Runge–Kutta integration scheme [43, 44] is employed as for all other terms in Equations (12) and (13a). To maintain at least second-order accuracy in time for the Crank-Nicolson scheme, each sub-time step requires the solution of a large linear system of equations that couples velocity and pressure.

The solution of this problem is iteratively found in a SIMPLE-type fashion [45, 46], i.e. by iteratively solving the Schur complement problem for the pressure. We employ a highly efficient commutation-based preconditioner for the pressure iteration, which was first employed by Elman [47] for steady-state problems. The preconditioner requires the solution of two subsequent Poisson-type equations in each pressure iteration cycle that we solve with the Krylov subspace method BiCGstab [48] combined with a geometric V- or F-cycle multigrid preconditioner [49]. Within multigrid we use lexicographically ordered Gauss–Seidel line relaxation for smoothing (cf. [50] for a general discussion on parallel smoothing techniques). The time integration of the velocity and the concentrations leads to Helmholtz-type equations, which are also solved with BiCGstab but do not normally require multigrid due to their better conditioning.

The simulation code (and in particular the multigrid preconditioner, cf. [51]) is designed for massively parallel supercomputers such that the present implementation scales easily beyond the order of $10^{11}$ grid points and $10^9$ processors on such machines [26]. More details on the algorithm and its implementation can be found in [25, 26]. An extensive validation of the code is documented in [26].
Figure 2. Salt concentration with isopycnal layer \( (c_{\text{sal}} = 0.75) \) around the freshwater inflow region at \( t = 250 \). White: freshwater \( (c_{\text{sal}} = 0) \), black: saltwater \( (c_{\text{sal}} = 1) \). The disturbed inflow leads to the formation of Kelvin–Helmholtz (K–H) vortices farther downstream. The vortices become unstable and break down into turbulence in the open basin (top), whereas they remain rather laminar in the confined channel (bottom).

6. Interaction of freshwater and ambient saltwater

We analyze the freshwater/saltwater mixing only for the statistically stationary state. As such a state was not reached in any of the laboratory experiments of McCool and Parsons [4] (probably due to practical limitations), we cannot directly compare our results with theirs. In addition, the initial transient cannot be compared either, because the exact initial conditions of the laboratory experiments are not documented. Hence, we can compare the results only qualitatively.

The interaction of the freshwater and the ambient saltwater (still without particles) is depicted in Figure 2 for the statistically steady state of both configurations. The pictures reveal that the basic two-dimensional K–H waves evolve at the interface and travel downwards up to \( x_1 \approx 20 \) in both configurations. The main differences between the two simulations are the different growth rates, final sizes and stabilities of the K–H billows. The Holmboe waves, which were observed in the experiments of McCool and Parsons [4], do not appear probably because our inflow profile favors the K–H instability.

The disturbances in the confined channel grow relative slow and reach only a small maximum amplitude. The small billow size and/or channel width seem to avoid secondary
instabilities, which could lead to the formation of larger 3D structures and thus to a more intense mixing between freshwater and saltwater. The fluid viscosity and the salinity diffusivity strongly damp the interface instabilities so that the flow remains rather laminar for most of the time.

Although the random disturbances of the interface at the boundary are exactly the same in the open basin, the K–H waves evolve much faster and saturate closer to the inflow. In addition, the absent confinement in the lateral direction triggers strong secondary instabilities of the K–H waves that contribute to their collapse farther downstream. We also observe that the billows are stretched in the lateral direction with growing distance to the inflow, which is obviously caused by the horizontal spreading of the freshwater plume. In addition, the flow must decelerate at the same time due to mass conservation and we observe that the K–H waves plunge deeper below the water surface before they collapse. As a result, the increasingly unstable stratification causes a quicker breakdown of the K–H billows into turbulence, which enhances the mixing of the freshwater with the ambient saltwater. We have already observed this in a previous study [29], in which this mechanism was even more pronounced due to smaller salinity Richardson numbers. The mixing of freshwater and saltwater in all other areas beyond the turbulent zone is much less dominated by turbulence rather than the diffusivity of the salinity.

Our excitation of the inflow is purely random in order to trigger disturbances of all wavelengths. To gain more information about disturbance group velocities in the symmetry plane \(x_2 = 0\) we investigate the first moment of the salinity distribution in the vertical direction,

\[
E_{\text{pot},3}^{\text{sal}} \equiv \int_0^{L_3} c_{\text{sal}} x_3 \, dx_3 ,
\]

which is equivalent to a potential energy per area. This quantity is plotted for \(x_2 = 0\) and in dependence of \(x_1\) and \(t\) in Figure 3. For the open basin we find that the propagation speed of the internal breaking K–H waves near the inflow, \(x_1 \lesssim 15\), is only slightly smaller than half of the freshwater bulk velocity at the inlet. The wavelengths as well as the vertical extents of these vortices are roughly equal to the inflow freshwater depth such that their temporal frequency is slightly smaller than 0.5. The waves at the interface between freshwater and saltwater directly behind the breakdown area (\(x_1 \gtrsim 30\)) are not of the K–H type and travel at a speed closer to the inflow freshwater speed, i.e. faster than the K–H vortices. However, the propagation speed slightly decreases with increasing distance to the inflow. The K–H waves in the confined channel are somewhat slower near the inflow compared to the open basin; however, they slightly accelerate farther downstream.

Next, we investigate the time-averaged velocity field \(\langle u \rangle \equiv \langle u \rangle_{250 \leq t < 550}\), from which the absolute value at the surface, \(x_3 = 4\), as well as the streamlines for the open basin are depicted in Figure 4. The far-field of the averaged surface flow is somewhat similar to that of a line source placed near the inflow. Moreover, the mean absolute velocity drops from 1.0 directly at the inflow to about 0.7 in the far-field, where it continues to decay only slowly farther downstream. This observation implies that the freshwater depth must decrease with increasing distance to the freshwater inflow due to the continuity constraint (Equation (13b), cf. Figure 2). For the confined channel (not shown) the streamlines are just straight lines parallel to the confinement and the velocity of the surface freshwater is more or less the same as the inlet bulk velocity.

Though we did not establish an explicit inflow boundary condition for ambient saltwater at the outflow, a weak backflow with \(|u| \ll 1\) beneath the freshwater/saltwater interface
Figure 3. $x_1$-t diagram of the potential energy per area, $E_{pot,3}^{sal}$, in the plane $x_2 = 0$. Black (white) corresponds to the minimum (maximum) of $E_{pot,3}^{sal}$. Generally, the disturbances in the confined channel (bottom) are much weaker than in the open basin (top); however, the group velocities are only slightly slower than in the open basin.

toward the freshwater inflow boundary can be observed (not shown here). Such an effect was also described in Maxworthy’s [12] experiments.

7. Particle transport

7.1. Integral quantities

For $t \geq 250$ the particles are added continuously to the inflowing freshwater. To get a better insight into the initial transient of the particle transport, we first investigate the mass of the suspended particles,

$$m_{part} \equiv R_{part} \int_{\Omega} c_{part} \, dV,$$  \hspace{1cm} (20)
Figure 4. Mean absolute velocity $|\langle u \rangle|$, $250 \leq t \leq 550$, and streamlines of $\langle u \rangle$ at the water surface, $x_3 = 4$. The mean velocity decays only slowly downstream such that the freshwater depth decreases correspondingly.

where the integration domain $\Omega$ is the entire computational domain. We find from Figure 5 that the particle masses level off at about $t \approx 310$, i.e. as soon as particles touch the ground for the first time. At about $t \approx 600$ the amount of particles is almost saturated in both basins. Particularly in the open basin the particle mass still continues to increase; however, at a much smaller rate than during the initial transient. In addition, the particle mass remains slightly unsteady. Because the imposed disturbances at the inflow are too small to account for this unsteadiness and the amount of particles that leave the domain via the outflow ‘O’ is negligible (as demonstrated below), we can conclude that the particle flux over the bottom of the basin must be responsible for the unsteadiness of the suspended particle mass.

The time derivative of the suspended particle mass is given by

$$\dot{m}_{\text{part}} \equiv \frac{dm_{\text{part}}}{dt} = Ri_{\text{part}} \int_{\partial \Omega} \left[ \frac{1}{Re Sc_{\text{part}}} \nabla c_{\text{part}} - (u + u^e_{\text{part}}) c_{\text{part}} \right] \cdot e^{\theta} \, dA, \quad (21)$$

Figure 5. Particle mass $m_{\text{part}}$ over time. The curves level off as soon as the particles touch the ground for the first time ($t \approx 310$). The statistically stationary state is reached at about $t \gtrsim 600$. 

Figure 6. Particle mass flux $\dot{m}_{\text{part}}$ over time. The fluctuations of the curve reveal that the vertical particle flux at the ground is unsteady, especially for the open basin. Almost all particles deposit on the ground inside the computational domains because $\dot{m}_{\text{part}}$ is about zero on the average for the statistically steady state.

which follows from the Gauss’ theorem ($\partial/\Omega$ denotes the integration area). We restrict the surface integral on the right-hand side of Equation (21) to the inflow plane ‘I’ and the bottom boundary ‘B’, respectively. As we find from Figure 6 that the average particle mass flux vanishes for late times, we can confirm that almost all particles deposit on the ground and do not leave the domain over the outflow ‘O’.

For the sake of completeness we also integrate the vertical particle mass flux over each horizontal plane independently (we drop the first term in Equation (21) for simplicity because its contribution is relatively small),

$$\dot{m}_{\text{part}}^{1,2}(x_3, t) \equiv R_{\text{part}} \int_0^{L_2} \int_0^{L_1} c_{\text{part}}(u + u_{\text{part}}^* \cdot e^g) \cdot e^g \, dx_1 \, dx_2,$$

(22)

and average this expression over time for the statistically steady state, i.e. we compute the time-average

$$\langle \cdot \rangle \equiv \langle \cdot \rangle_{600 \leq t \leq 1600}$$

(23)

of $\dot{m}_{\text{part}}^{1,2}$ (cf. Figure 7). The averaging operation (Equation (23)) is used also for all subsequent temporal averages. Although $\langle \dot{m}_{\text{part}}^{1,2} \rangle$ is not perfectly converged yet, it clearly illustrates that the vertical particle flux at each altitude $x_3$ is about the same as the total inlet flux, except for the interval $3 \lesssim x_3 \lesssim 4 = L_3$, in which the inlet is established. We will return to the quantity $\dot{m}_{\text{part}}^{1,2}$ at the end of Section 7.4.

So far we have only investigated the integral development of the particle suspension. To also assess its spatial distribution, we compute the potential energy of the particle suspension,

$$E_{\text{part}}^{\text{Pot}} \equiv R_{\text{part}} \int_{\Omega} c_{\text{part}} x_3 \, dV,$$

(24)
Figure 7. Average vertical particle mass flux with respect to $x_3$ for the statistically steady state. The plot illustrates that the vertical mass flux remains constant below the inlet altitude $x_3 \approx 3$ because almost all particles deposit on the ground within the computational domain.

from which we derive its center of mass in the vertical direction,

$$x_{3,\text{part}}^c \equiv \frac{E_{\text{pot,part}}}{m_{\text{part}}}.$$  \hspace{1cm} (25)

We find from Figure 8 that the potential energies level off at about the same time as the masses of the suspended particles $m_{\text{part}}$. Beyond that point, particle masses and potential energies are not anymore proportional to each other because the centers of mass gradually move toward the basin half-height $x_3 = 2$ (cf. Figure 8). A clear difference between the two configurations is the final magnitude of the potential energy: It is much larger for the open basin, although the final amount of suspended particle mass is roughly the same for both cases.

As mentioned in Section 1 we expect that turbulence enhances the particle settling velocity compared to the Stokes settling velocity. Turbulence is mostly driven by the kinetic energy of the freshwater inflow but the potential energy of the particles can also be released in additional advective motion. This contribution is small, as indicated by the small particle Richardson number $R_{i,\text{part}}$, and the results in Figure 8 show that this additional energy source saturates as soon as the statistically steady state is reached.

At early times $t > 250$, the center of mass for the open basin simulation exceeds the center of mass for $t = 250$, $x_{3,\text{part}}^c \approx 3.5$ (cf. Equation (16)), which implies that the particles are initially lifted to higher altitudes and spread in the horizontal directions due to mass conservation. Subsequently, they rapidly settle at rates that are on the order of the Stokes settling velocity, indicated by the time derivative of the center of gravity (cf. Figure 8). Therefore, the particles must settle in this period at least with the Stokes settling velocities plus this (integral) velocity. Finally, the center of mass reaches a slightly larger altitude than the basin’s half-height, which indicates that somewhat more particles are located in the upper half of the basin.

In the confined channel simulation the particles start to settle from the beginning without any initial lifting. Another fundamental difference to the open basin is the significantly lower center of mass at any time. The reason for this difference becomes more clear if we more qualitatively compare the spatial particle distributions in both simulations.
7.2. Spatial particle distribution over time

To get a better idea of the settling processes we visualize two exemplary slices through the domains, $x_2 = 3$ (Figures 9 and 10) and $x_1 = 26$ (Figures 11 and 12), respectively, at different times, $t = 300, 350, 400$ and $600$.

In the area close to the inflow of the open basin, the particle concentration is transported more or less passively with the carrier fluid. As soon as the particles have traveled beyond the K–H vortex breakdown area, their transport speed decelerates due to the spreading of the freshwater current such that inertial forces become less dominant. Consequently, the density difference, the diffusion and the Stokes settling velocity of the particle concentration play a more important role outside the turbulent areas. This is also the location where most of the particle discharge occurs from the near-surface particle plume. This plume is established in the vicinity of the freshwater/saltwater interface close to the water surface.

These observations are different for the confined channel. As no K–H vortex breakdown and also no significant deceleration of the freshwater current is present, the particle concentration expands much farther downstream than in the open basin. Moreover, the particles settle out of the initial near-surface particle plume over its entire length and not only in certain areas. The particle concentration is also much larger than the earlier one.
Figure 9. Particle concentration in the plane \( x_2 = 3 \) of the open basin. White: clear fluid \((c_{\text{part}} = 0)\), black: maximum particle concentration \((c_{\text{part}} = 1)\). From top: \( t = 300, 350, 400, 600 \). After passing the K–H breakdown \((t = 300)\), the particles initially settle by forming sheets and fingers \((t = 350)\). The area beneath the near-surface particle plume is filled gradually \((t = 400)\) until the statistically steady state is reached \((t \geq 600)\). The settling processes becomes increasingly disordered after \( t \gtrsim 350 \).

Figure 10. Particle concentration in the plane \( x_2 = 3 \) of the confined channel. Color bar and further description is given in Figure 9. The initial particle settling mechanisms are about the same as for the open basin. However, the particle concentration is much larger and finally fills almost the entire channel. In addition, the mixing with clear ambient fluid is much less pronounced.
such that a distinct near-surface particle plume is not present for late times as in the open basin.

From the same pictures one can observe sheet/finger-like settling convection at early times ($t \approx 350$), which could be categorized somewhere between ‘mixing-induced convection’ [6] in the experiments of Maxworthy [12] (Figure 3) and ‘finger convection’ in the experiments of Parsons et al. [6] (Figure 3) and McCool and Parsons [4] (Figures 3 and 4). Stages of sheet convection were explicitly mentioned in Parsons et al.’s [6] experiments (Figure 6). These structures are initially more or less two-dimensional and sheet-like as shown in Figures 13 and 14, where iso-surfaces of the particle concentrations are depicted from below. Moreover, the structures are aligned with the direction of the surface streamlines, cf. Figure 4 for the open basin. We suspect that finger settling convection is sensitive to shear stresses that are caused by the transversal freshwater current at the surface and the saltwater backflow underneath. However, if the particles concentrate along streamlines of the transversal flow, then shear stresses act only in planes parallel to the sheets and the particles can still take an enhanced settling mode by spreading in directions that are normal to the sheets. Correspondingly, the sheets become more three-dimensional and finger-like as soon as they pass the areas with larger shear stresses. However, the sheet-/finger-like convection mode is accentuated only around $t \approx 350$.

At later times (i.e. close to the statistically steady state) the horizontal extent of the particle plume is more or less the same as for the transient phase. However, the amount of suspended particles has increased significantly. The particle plume is not a thin layer in

Figure 11. Particle concentration in the plane $x_1 = 26$ of the open basin. Left column $t = 300, 350$; right column $t = 400, 600$. Color bar and further description are given in Figure 9.
Figure 13. Isopycnal layer \((c_{\text{part}} = 0.25, \text{view from below})\) of the particle concentration in the open basin at times (from top) \(t = 300, 350, 400\) and 600. Further description is given in the caption of Figure 9.
the freshwater/saltwater interface anymore but now fills almost the entire water depth. The settling process also becomes increasingly disordered. In addition, we observe a so-called nepheloid layer on the bottom of the open basin simulation, which is formed by slower settling particles, cf. Figure 11 at \( t = 600 \) and Section 7.4. Such layers were also reported in McCool and Parsons’s [4] experiments.

7.3. Average particle settling velocity

To shed light on the enhancement of the particle settling, we define the average particle settling velocity in gravity direction \( e_\| \),

\[
\bar{u}_{\text{part}} \equiv \frac{\int_{\Omega} c_{\text{part}} (u + u_{\text{part}}^g) \cdot e_\| \, dV}{\int_{\Omega} c_{\text{part}} \, dV},
\]

sometimes also referred to as ‘effective settling velocity’, cf. e.g. [8]. The result of this expression strongly depends on the integration domain \( \Omega \) because the various areas of the physical domain will contribute quite differently (cf. the discussion in the last paragraph of this section and Figure 16). Especially the dense particle suspension in the inflow region is mainly advected in the horizontal directions due to the dominant freshwater momentum, whereas the vertical movement is much smaller. Figures 9 and 11 suggest that the average settling velocity near the water surface is small in contrast to the region beneath the freshwater/saltwater interface. Similarly, the particles in the nepheloid layer close to the bottom settle only about with the particle Stokes settling velocity, cf. Section 7.2. Therefore, we integrate over the entire horizontal plane but vertically only over the layer \( 1 \leq x_3 \leq 2 \) to exclude most of the slowly settling particles in other areas and to demonstrate a notable increase of the particle settling speed compared to the pure Stokes settling velocity.

These results are plotted in Figure 15. We find for both configurations that the particle settling velocity is most enhanced around \( t \approx 310 \ldots 350 \), where the sheet/finger convection occurs (cf. the discussion in Section 7.2 and Figures 9–14). The relative enhancement of the settling velocity attains up to 500\% for the open basin and 150\% for the confined channel, which was already indicated by the temporal development of the vertical center of mass.
Figure 15. Relative enhancement of the particle settling velocity over time. The absolute average settling velocities \( |u_{\text{part}}^{\text{av}}| \) are maximal during the finger/sheet convection phase around \( t \approx 310 \ldots 350 \). The Stokes settling velocity \( |u_{\text{part}}^{S}| \) is also exceeded in the statistically steady state regime, however, only for the open basin configuration.

(cf. Section 7.1 and Figure 8). When the statistically stationary state is reached, the average settling velocity is still larger than the Stokes settling velocity; however only for the open basin where the gain is roughly between 30% and 60%. For the confined channel the settling enhancement vanishes almost completely.

Our nondimensional average settling velocities for the initial transient correspond to (dimensional) average settling velocities of 0.9 cm/s and 0.4 cm/s, respectively, for the parameters given in Table 1. This agrees roughly with the measurements of McCool and Parsons [4], who observed average settling velocities of about 1–2 cm/s. However, it is necessary to remark – in addition to the comment made at the beginning of Section 6 – that a serious comparison between the results is not feasible for two reasons: first, most of our parameters (and especially the Reynolds number) are not exactly the same as in the experiments due to our technical limitations and second, the informations on the measured particle settling velocities of the laboratory measurements are relatively rough and narrow.

As mentioned above, the average particle settling speeds of our simulations are expected to vary with the vertical position of the measurement. To illustrate this, we compute the integrals in Equation (26) over each horizontal plane independently,

\[
\begin{align*}
    u_{\text{part}}^{\text{av,1,2}}(x_3, t) & \equiv \int_0^{L_2} \int_0^{L_1} c_{\text{part}}(u + u_{\text{part}}^x) \cdot e^s \, dx_1 \, dx_2 \bigg/ \int_0^{L_2} \int_0^{L_1} c_{\text{part}} \, dx_1 \, dx_2.
\end{align*}
\]  

(27)

The time-average of \( u_{\text{part}}^{\text{av,1,2}} \) for the statistically steady state is depicted in Figure 16. We find that the settling speed is maximal slightly below the basin half-height, \( x_3 = 2 \), for the open basin and at about \( x_3 = 3 \) for the confined channel. In addition, the near-surface particle plume in the open basin settles only very slowly, even slower than the Stokes settling velocity. The amplitudes in the interval \( 1 \leq x_3 \leq 2 \) (which was used to compute \( u_{\text{part}}^{\text{av}} \) in Figure 15) confirm the results of Figure 15.
Figure 16. Average relative enhancement of the particle settling velocity with respect to \( x_3 \) for the statistically steady state. The area of enhanced particle settling beneath the near-surface particle plume is clearly visible for the open basin. The near-surface particle plume settles only very slowly. These observations do not apply for the confined channel configuration.

7.4. Correlation between turbulence, availability of clear ambient fluid and enhanced particle settling

To assess the correlation between particle settling enhancement and turbulence, we investigate the root mean square (RMS) of the velocity fluctuations \( u' \equiv u - \langle u \rangle \),

\[
\sigma_{u'_{RMS}} \equiv \langle (u' \cdot u')^{\frac{1}{2}} \rangle,
\]

which acts as a simple measure for the local turbulence intensity. Equation (28) is computed for the plane \( x_2 = 3 \) and the statistically stationary state. The results are depicted in Figure 17 for both configurations. Generally, we find that \( \sigma_{u'_{RMS}} \) is significantly larger for the open basin and, moreover, the turbulent motion is limited to the area in which the particle settling takes place (cf. Figure 18, where the average particle concentrations \( \langle c_{\text{part}} \rangle \) are depicted for the same plane and time interval). For the confined channel this correlation is less pronounced than in the open basin and at the same time the average particle settling enhancement is almost negligible.

Generally, the fact that the particles settle faster in the presence of turbulence is in good agreement with other rather idealized numerical and laboratory experiments (e.g. [9–11, 36] for homogeneous isotropic turbulence). However, the major difference between these studies and ours is the neglected particle inertia (expressed by the particle Stokes number) in our simulations. Such a particle model was not investigated in the cited studies, but our results clearly demonstrate that (at least in our configurations) the particle inertia is not an essential feature to obtain an average particle settling speed larger than the individual settling speed.

Maxey et al. [38] used the same particle model in Lagrangian description as we have done (cf. Equations (7) and (10)); although they investigated the particle settling in homogeneous isotropic turbulence. From their analysis it is clear that the particles must settle exactly at the Stokes settling velocity on the average, independent of the turbulence intensity. The same can be observed for the confined channel in our study: The particles settle only with the Stokes settling velocity in the statistically stationary regime.
A significant difference between the open basin and the confined channel configuration concerns the mixing of the particle plume with clear ambient fluid. The confinement in the latter configuration strongly prohibits the mixing of these two phases because the separation/contact area between clear fluid and particle-laden fluid is smaller than in the open basin. In the confined channel this mixing zone is limited to the end of the particle plume, whereas the entire longitudinal length of the particle plume is additionally available in the open basin. Therefore, the particle settling enhancement is also significantly influenced by the availability of clear ambient fluid to the particle plume. Without this feature the potential energy of the particle suspension cannot be released into additional kinetic energy, which may ultimately enhance its settling speed.

Summing up, we explain the observed settling enhancement as follows: The particle suspension is fed into the basin close to the water surface from where the particle suspension can settle (under appropriate conditions) with speeds on the order of the buoyancy velocity of the suspension, \( \sqrt{\tilde{g} \tilde{h}} \) in dimensional quantities or \( \sqrt{R_i \tilde{h}} \) in nondimensional form. The buoyancy velocity can be much larger than the individual particle Stokes settling velocity \( \tilde{u}_{\text{part}} \) or \( u_{\text{part}} \), which can explain large enhancements of the settling velocities. Obviously, the open basin configuration provides such ‘appropriate’ conditions, namely the presence of turbulence and a large mixing zone for particles and clear ambient fluid, which ultimately leads to sustained average settling velocities larger than the Stokes settling velocity.

Finally, we would like to comment briefly on the form of the average particle plume \( \langle c_{\text{part}} \rangle \) in the open basin (cf. Figure 18): as soon as the particles have reached the statistically steady state, the particle flux from the inlet to the bottom of the basin is constant, as demonstrated in Section 7.1 and Figure 7. Next, we observed average enhanced particle settling speeds (cf. Section 7.3 and Figure 16), which were most pronounced near the basin half-height, whereas the particles close to the water surface (near-surface plume) and in the vicinity of the bottom (nepheloid layer) settled only at speeds which were on the order of the Stokes settling velocity or even smaller. Therefore, the average particle plume must be contracted horizontally in the area of large settling enhancements due to the fluid incompressibility. This horizontal contraction is slightly visible in Figure 18 for the open basin. To better illustrate this effect, we independently integrate the particle concentration
Figure 18. Average particle concentrations $\langle c_{\text{part}} \rangle$ in the plane $x_2 = 3$. White: clear fluid ($c_{\text{part}} = 0$), black: maximum particle concentration ($c_{\text{part}} = 1$). Top: open basin, bottom: confined channel. For the open basin the particles are located in the same area where also the largest velocity fluctuations occur, indicating a correlation between enhanced particle settling and turbulence. This correlation is less pronounced for the confined channel.

in each horizontal plane,

$$dm_{\text{part}}^{1,2}(x_3, t) \equiv Ri_\text{part} \int_{x_1}^{L_2} \int_{x_1}^{L_1} c_{\text{part}} \, dx_1 \, dx_2 = \frac{m_{\text{part}}^{1,2}}{u_{\text{us,av},1,2}^{\text{part}}}. \quad (29)$$

The time-average of this differential particle mass for the statistically steady state is depicted in Figure 19 (note that $\langle dm_{\text{part}}^{1,2} \rangle = \langle m_{\text{part}}^{1,2} / u_{\text{us,av},1,2}^{\text{part}} \rangle$ and $\langle m_{\text{part}}^{1,2} \rangle / \langle u_{\text{us,av},1,2}^{\text{part}} \rangle$ are almost identical in the present case). The plot nicely depicts the particle plume contraction that is most pronounced in the basin half-height and the distinct near-surface particle plume. These features are not present for the confined channel because the particle settling speed is not significantly enhanced.

Figure 19. Average differential particle mass with respect to $x_3$ for the statistically steady state. The contraction of $\langle dm_{\text{part}}^{1,2} \rangle$ in the vicinity of the basin half-height, $x_3 = 2$, is the result of the enhanced particle settling speed in these areas. The near-surface particle plume at about $x_3 \approx 3.5$ is clearly visible. Both features are only present for the open basin configuration.
Figure 20. Temporal maxima of the absolute fluid acceleration $\max_t |\partial u(x, t)/\partial t|$ for the statistically steady state, $600 \leq t \leq 1600$. Top: open basin, bottom: confined channel. The maximum fluid acceleration indicates whether or not the particle inertia plays an important role in the particle model, Equation (6).

8. A posteriori verification of the particle model

Having analyzed and compared the flow and the particle settling for the two configurations, we return to the applicability of the particle model. As explained in Section 3, we neglected the particle inertia in both simulations because we assumed that the particle inertia is small compared to the buoyancy forces. To check this a posteriori we compute the temporal maxima of the absolute fluid acceleration, $\max_t |\partial u(x, t)/\partial t|$, for the statistically steady state ($600 \leq t \leq 1600$), which provides an estimate for the upper limit of the expression in Equation (9). As we find from Figure 20, the maximum fluid acceleration reaches magnitudes on the order of one to ten in the K–H vortex breakdown area so that the contribution of the particle inertia in Equations (6) and (8) is at most on the order of $2St^{20}$ according to Equation (9). Considering the values of $u_{\text{part}}^s$ and $St$ given in Table 1, we can conclude that the contribution of the particle inertia in Equation (8) could be of the same order as the Stokes settling velocity $u_{\text{part}}^s$ locally in certain confined areas of the computational domain. However, the fluid acceleration is much smaller for the rest of the domain such that the particle acceleration is obviously not an important part of the model as long as we are only interested in the settling beneath the near-surface particle
plume. Nevertheless, one can suspect for instance that the particle inertia could play a more important role for the horizontal extents of the near-surface particle plume.

9. Conclusions

We presented two numerical simulation setups (cf. Figure 1) and some initial results of highly resolved simulations of laboratory-scale estuary flows. The results were obtained by DNS, which are principally limited to such model problems due to their high numerical effort. The main advantage of DNS is that it allows very accurate and detailed investigations of basic effects. The study’s objective was to investigate the mixing of freshwater with ambient saltwater and the effect of turbulence on the settling speed of suspended particles. The results were compared qualitatively with experimental findings, especially with the results of McCool and Parsons [4].

To this end we first introduced the relevant flow parameters, discussed typical values for these parameters and investigated their implications on the governing equations and the numerical model, respectively. To permit high-resolution numerical simulations of our target configurations and to distinguish between different competing effects (cf. the discussion on particle settling enhancement, Section 3, for instance) we introduced a number of simplifications in our numerical model. Most of our assumptions are straightforward (e.g. a non-deformable water surface, advective outflow boundaries, Boussinesq approximation and higher diffusivity of the salinity and of the particle suspension) and can be expected to influence our results only marginally. On the other hand, we also neglected the inertia of individual particles and kept only their buoyancy forces (expressed by the Stokes settling velocity, $u_{\text{part}}$, and by the Richardson number of the particle suspension, $Ri_{\text{part}}$). To justify this assumption we performed an a posteriori check using our results that indicated that the particle inertia would probably have only a small effect on the results in the relevant spatial areas.

We conducted two simulations that differ only in the geometry of the model configuration (cf. Figure 1): the first (‘open basin’) is geometrically close to a realistic estuary, in which lateral spreading of the flow is permitted, whereas this lateral spreading is prohibited in the second configuration (‘confined channel’). To enhance the convective mixing of different species we triggered K–H vortices in the freshwater/saltwater interface using an appropriate inflow profile. We found at least for the open basin that these K–H waves collapse farther downstream and provide a source of turbulent motion. In addition, the particle concentration transports potential energy into the basin, which can be released into turbulence and into an enhanced particle settling, but only under certain conditions.

Generally, the basic particle settling mechanisms of the experiments [4, 6, 12], i.e. sheet/finger settling convection and turbulence-enhanced particle settling, can also be observed in our simulations. Furthermore, we found average particle settling speed enhancements, which are roughly of the same order as the laboratory measurements. Particularly, we found transient settling enhancements of up to 500% for the open basin and up to 150% for the confined channel. As soon as the flow reached a statistically steady state, these numbers dropped to 30–60% for the open basin and to essentially zero for the confined channel. We emphasize that the latter numbers cannot be compared to the corresponding laboratory experiments directly because statistically steady states were not reached in these studies, possibly due to technical limitations.

As not only the settling enhancement but also the turbulence intensity is generally larger in the open basin, we can confirm that the average particle settling speed correlates with the turbulence intensity. Our observations were made in relatively realistic flow
configurations, nevertheless they are also in good agreement with other numerical and laboratory experiments of homogeneous isotropic turbulence, e.g. [10, 9, 11]. However, the settling enhancements in these studies were due to the particle inertia, which was not considered in our simulations. Without particle inertia, no settling enhancement can be expected for homogeneous isotropic turbulence, as demonstrated by Maxey et al. [38]. This can be confirmed for the statistically stationary state in our confined channel configuration. On the other hand, the results for the open basin clearly demonstrate that (at least for this particular configuration) particle inertia is not an essential feature to obtain sustained average particle settling speeds larger than the individual particle settling speed under the influence of turbulence.

Besides the smaller turbulence intensity, we also observed that the mixing of the particle plume with clear ambient fluid is much less pronounced in the confined channel because the separation/contact area between clear fluid and particle-laden fluid is much smaller than in the open basin. Hence, the particle suspension in the confined channel is locally much more homogeneous, such that the potential energy of the particle suspension cannot be released into additional kinetic energy, i.e. a settling velocity larger than the Stokes settling velocity is not feasible. However, particle inertia, for instance, could lead to a self-sustaining heterogeneous particle distribution and thus to enhanced particle settling in such cases.

Therefore, we conclude that the approximate upper limit for the particle settling speed, the buoyancy velocity of the particle suspension, can only be approached if vertical concentration gradients of the particle suspension can be maintained. To provide such gradients in the absence of particle inertia, the particle suspension is needed to be mixed convectively with clear ambient fluid. The convective motion can be provided by turbulent motion.

We plan to conduct further simulations with different parameter values in the future. Particularly, we are interested in studying the influence of the Reynolds number, which is currently smaller than in real estuary mouth flows. To this end it might be necessary to switch to LES.

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