Particle deposition in turbulent square duct flows

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Abstract. Particle deposition in fully developed turbulent square duct flows is predicted using large eddy simulation for Reynolds numbers, based on the bulk flow velocity and duct width, equal to 250k, 83k and 10,320. A particle equation of motion, solved in conjunction with a Lagrangian particle tracking technique, and including Stokes drag, lift, buoyancy and gravitational forces is used to analyse the trajectory of 50, 100 and 500 μm particles. Results obtained for the fluid phase show good agreement with experimental data and the predictions of direct numerical simulations. Predictions for particles show that high-inertia particles (Stokes number, St > 12.38) tend to deposit close to the corners of the duct floor, while low-inertia particles (St < 6.43) deposit near the floor centre. Particle deposition in the vertical direction is also found to increase with flow Reynolds number, whilst in the horizontal direction deposition increases with particle size and decreases with Reynolds number. Additionally, and in both the vertical and horizontal directions, the deposition profile, as quantified by the probability density function of deposited particle locations, is more variable for small particles when compared to larger ones, independent of the flow Reynolds number.

1. Introduction
Particle deposition in wall-bounded flows has been widely studied over the last fifty years, and numerous investigations have enhanced our understanding of particle dispersion and deposition. Most of the computational studies performed have focussed on homogeneous and isotropic turbulent flows in periodic domains (e.g. Squires & Eaton 1991), although inhomogeneous turbulent flows, as occur in circular pipes and plane channels, have also been considered (e.g. Brooke et al. 1994). Brooke et al. (1994) examined the free-flight mixing and deposition of aerosol particles using direct numerical simulation (DNS) of a channel flow, finding that particles deposit in one of two ways: diffusion or free-flight towards the wall. The latter was seen as the principal mechanism since deposition was dominated by particles starting free-flight at large distances from the surface. However, observing the accumulation of particles near the wall, these authors noted the possibility of particle deposition due to diffusive processes. Subsequently, they used their results to demonstrate that an enhanced deposition rate could be attributed to the inertia-dependent transport of particles from the core of the channel to the near-wall region, where they tended to concentrate. Despite such research, however, further work is necessary to elucidate the mechanisms by which particles deposit in inhomogeneous turbulent flows. Of interest in this work, due to its practical relevance, are flows in horizontal square ducts.

A number of studies have examined turbulent single-phase flows in square ducts, including experimental investigations (e.g. Brundrett & Baines 1964; Gessner et al. 1979), direct numerical simulations (e.g. Huser & Biringen 1993) and large eddy simulations (e.g. Winkler et al. 2006). All these investigations have demonstrated that turbulence-driven secondary motions that arise in the
plane of the duct cross-section act to transfer fluid momentum from the centre of the duct to its corners. They have also established that the Reynolds normal and shear stresses contribute equally to the production of mean streamwise vorticity. In contrast to the body of work on single-phase flows, there exist few studies of particle-laden turbulent flows in ducts. Winkler et al. (2006) did, however, apply large eddy simulation (LES), coupled with Lagrangian particle tracking, to study particle deposition in a duct flow, focusing on particles with response times in the range $\tau_s = 0.072-256.32$. Sharma & Phares (2006) also used DNS to study secondary flow effects on particle transport in a duct flow, although the effects of gravity were neglected. Both of these works focused on low Reynolds number turbulent flows ($Re_z = 360$ and $300$, respectively, based on the mean friction velocity and duct width). More recently, the present authors applied LES to study particle dispersion (Fairweather & Yao 2009) mechanisms in a duct flow at high Reynolds number ($Re_z = 10,500$). Clearly, given the limited amount of research, the particle deposition mechanism in duct flows has not been fully elucidated across the wide range of flow Reynolds and particle Stokes numbers of practical relevance.

In this study particle deposition in fully developed turbulent square duct flows is investigated for a range of Reynolds numbers (10k-250k), particle sizes (50-500 $\mu$m) and associated Stokes numbers (0.07-1866). Predicted flow fields are compared with available experimental data and DNS results, with results for particles demonstrating the principles of deposition in these flows.

2. Mathematical model

The flow considered was three-dimensional and described using a Cartesian co-ordinate system, with the $z$ axis aligned with the streamwise direction, the $x$ axis with the direction normal to the duct floor, and the $y$ axis with the spanwise direction. The corresponding velocity components in the $(x, y, z)$ directions are $(u, v, w)$, respectively. The boundary conditions for the momentum equations were no-slip at the walls, and the specification of inflow and outflow conditions at the open boundaries of the duct was avoided by assuming that the instantaneous flow field was periodic along the streamwise direction, with the pressure gradient adjusted dynamically to maintain a constant mass flux. The Navier-Stokes equations were solved numerically in a domain of size $h \times h \times 4\pi h$ in the $x$, $y$ and $z$ directions, respectively. The physical domain was discretised using between $4.5 \times 10^5$ grid points for the low Reynolds number simulation, and $5.9 \times 10^5$ grid points for the high Reynolds number case. All discretisations were uniform in the streamwise direction, whereas in the vertical and spanwise directions grid points were clustered towards the walls. Other simulations using an increased total number, and alternative distributions, of nodes were also used to give better resolution near the walls of the duct, further details of which can be found in Fairweather & Yao (2009). These sensitivity studies demonstrate that the discretisations employed resulted in turbulence statistics that were independent of grid resolution. The flows investigated had bulk Reynolds numbers, $Re_b = w h^2 / \nu$, of 250k, 83k and 10,320, defined using the cross-stream area-averaged streamwise velocity, with equivalent friction Reynolds numbers, $Re_* = u_* h / \nu$, of 10,500, 3860 and 600.

The LES used a top hat filter to decompose the Navier-Stokes equations. This decomposition was applied to the conservation equations, assuming an incompressible Newtonian fluid with constant properties, giving rise to terms which represents the effect of the sub-grid scale (SGS) motion on the resolved motion. The SGS stress model used was the dynamic model of Germano et al. (1996), implemented using the approximate localization procedure of Piomelli & Liu (1995) together with the modification proposed by di Mare & Jones (2003). This model represents the SGS stress as the product of a SGS viscosity and the resolved part of the strain tensor, and is based on the possibility of allowing different values of the Smagorinsky constant at different filter levels. Test-filtering was performed in all space directions, with no averaging of the computed model parameter field. Computations were performed using the computer program BOFFIN. The code implements an implicit finite-volume incompressible flow solver using a co-located variable storage arrangement. Because of this arrangement, fourth-order pressure smoothing is applied to prevent spurious oscillations in the pressure field. Time advancement is performed using an implicit Gear method for all transport terms, and the overall procedure is second-order accurate in space and time. The time step

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is chosen by requiring that the maximum Courant number lies between 0.1 and 0.3, enforced for reasons of accuracy. Further details of the mathematical model employed, and the numerical algorithm and its implementation, may be found elsewhere (di Mare & Jones 2003; Fairweather & Yao 2009).

Given the flow field information derived from the LES, particle motion was subsequently tracked using a Lagrangian technique (Fan et al. 2002) in which the particles are followed along their trajectories through the unsteady, non-uniform flow field. The flow was assumed to be dilute, with no particle-particle interactions, and one-way coupled, thereby neglecting the effect of particles on the fluid. All particles were taken to be rigid spheres with identical density and diameter, with elastic particle-wall collisions. The motion of the particles is governed by a force balance equation, and in this work this equation was solved accounting for the Stokes drag, lift, buoyancy and gravitational forces. A fourth-order Runge-Kutta scheme was used to solve the equation of motion, given the initial particle location and velocity. The initial particle positions were distributed randomly throughout the duct, corresponding to an initially uniform wall-normal particle number density profile. Particles were assumed to interact with turbulent eddies over a certain period of time, that being the lesser of the eddy lifetime and the transition time. For particles leaving the duct in the streamwise direction, periodic boundary conditions were used to reintroduce them into the computational domain. The total number of particles within that domain was sufficient to ensure statistical independence of the results.

Particle and fluid densities were set to 2.5 kg m$^{-3}$ and 1 kg m$^{-3}$, respectively, with the kinematic viscosity of the fluid $1.004 \times 10^{-6}$ m$^2$ s$^{-1}$. The particle relaxation time is $\tau_p = \rho_p d_p^2/(18 \mu f_0)$, where $f_0 = 1 + 0.15Re_p^{0.657}$. The non-dimensional particle response time is defined as the particle Stokes number, $St = \tau_p u_s/\nu$, where the $u_s$ is the shear velocity $(u_s = (\tau_w/\rho)^{1/2}$, with $\tau_w$ the wall shear stress). Three particle diameters were considered, namely $d_p = 50$, 100 and 500 µm, with corresponding particle Stokes numbers of 5.92, 3.23 and $7.71 \times 10^3$ (50 µm), 89.77, 12.38 and 0.30 (100 µm), and 1866.82, 287.26 and 6.43 (500 µm), in the $Re_\mu = 250k$, 83k and 10k flows, respectively.

3. Results and discussion

To determine the accuracy of the simulation approach, LES of turbulent flow in a duct was performed and compared with available data and DNS, with the results shown in figure 1. Solutions at $Re_\mu = 250k$, 83k and 10k are compared with the experimental data of Gessner et al. (1979) and Po (1975) at $Re_\mu = 250k$, and Brundrett & Baines (1964) at $Re_\mu = 83k$, and with the DNS of Huser & Biringen (1993) at $Re_\mu = 10k$. The effect of Reynolds number on the streamwise mean velocity shown in this figure, which gives velocities normalized by the bulk flow velocity along the lower wall bisector ($y/h/2$), shows good agreement between the simulations and the results of the alternative studies.

Considering particle deposition in the (vertical) $x$-direction, figure 2(a-c) shows results for the $Re_\mu = 250k$ flow in terms of the probability density function (pdf) of the location of the particles on the floor of the duct (non-dimensional horizontal distance, $y^+$). Results are shown at different times ($t^+$) and for each particle size. It is seen that for the smallest 50 µm ($St=5.92$) particles the deposition appears highly variable. The accumulation of deposited particles is also seen to increase with particle size. In addition, and with the progress of deposition, the smallest particles tend to preferentially deposit close to the centre of the floor, while the medium sized and largest particles tend to deposit more efficiently near the side walls of the duct (at $y^+=\pm 5275$), this being particularly the case for the 500 µm ($St=1866.82$) particles. In the $Re_\mu = 83k$ flow (figure 2(d-f)), it only takes a short time ($t^+ < 20000$) for most (>90%) of the largest 500 µm ($St=287.26$) particles to deposit on the floor of the duct, while for the 50 µm ($St=3.23$) particles the deposition rate is still as low as 5% at $t^+ = 29,897$. Again, it is seen that the particle pdfs become more variable as the particle size decreases, similar to what was observed in the $Re_\mu = 250k$ flow. Also, and again similar to the latter flow, particle accumulation near the side walls can be seen at later times for both the 100 µm ($St=12.38$) and 500 µm ($St=287.26$) particles, while the smallest particles tend to accumulate towards the centre of the floor. Differences do arise between the $Re_\mu = 250k$ and 83k flows due to the Reynolds number effect. In figure 2(d-f), therefore, the 500 µm ($St=287.26$) particles are seen to accumulate near the side walls at $t^+ = 11,211$, while in the higher Reynolds number flow this does not occur until $t^+ = 362,805$. Deposition
of these particles near the side walls therefore occurs earlier in the lower Reynolds number flow, which is due to particle deposition being in general more rapid in this case. At large times, however, particle deposition in the \( Re_b=83k \) flow shows less of a tendency for the particles to accumulate either at the side walls or at the centre of the floor, with a more even distribution across the floor apparent. Figure 2 (g-i) gives particle deposition pdfs for \( Re_b=10k \). As noted for the higher Reynolds number flows, deposition is more variable for the smallest particles, although the distribution of the deposited particles is similar for the 50\( \mu m \) (\( St=0.07 \)) and 100\( \mu m \) (\( St=0.3 \)) cases, with their pdfs being of comparable magnitude. For the 500\( \mu m \) (\( St=6.43 \)) particles, however, and at variance with earlier observations, in the \( Re_b=10k \) flow deposition occurs preferentially near the centre of the duct floor. It should be noted that preferential deposition near the side walls of the duct was never observed for any of the particle sizes considered within this flow. In fact, for the largest \( St=6.43 \) particles, figure 2 (i), and at all times considered, deposition almost never happened close to the side walls. This finding is in line with that of Winkler et al. (2006) who used LES of a duct flow at \( Re_b=5,810 \) to investigate deposition at \( St=0.072-256.32 \), noting preferential deposition at the wall centre with little in the duct corners. Results for this particular flow are also in line with those of Phares and Sharma (2006).

Figure 3(a-c) shows results for particle deposition in the \( y \)-direction for the \( Re_b=250k \) flow. At the times considered, the deposition ratios were: for the 50\( \mu m \) and 100\( \mu m \) particles, 2\%, 5\% and 9\%; and for the 500\( \mu m \) particles, 3\%, 5\% and 21\%. Compared to the \( x \)-direction, deposition is clearly low in the \( y \)-direction due to the differing deposition mechanism. Similar to results in the \( x \)-direction, however, the 50\( \mu m \) particles have a more variable deposition profile at early times when compared to the other particles. Under the influence of gravity, all particles also show, with time, preferential deposition close to the bottom of the wall (at \( x^+=5275 \)), with this trend increasing with particle size. Comparing the results of figure 2(a-c) and 3(a-c) allows further analysis of the way in which particles deposit in the \( x-y \) plane. Clearly, from figures 2(c) and 3(c), and at \( t^+=362,805 \), the 500\( \mu m \) particles not only deposit at the side walls (\( y^+=5275 \)) but also settle towards the bottom of those walls (\( x^+=5275 \)), thereby demonstrating preferential deposition in the duct corners. At the same time, figures 2(b) and 3(b) indicate a preferential deposition at similar sites for the 100\( \mu m \) particles, although not to the same extent as for the largest particles. For the 50\( \mu m \) particles, figures 2(a) and 3(a), although the latter figure shows a tendency for particles to deposit towards the bottom of the side wall, clearly from figure 2(a) these particles are more prone to accumulate towards the centre of the floor. This tendency for large particles to deposit in the duct corners has been noted previously (Phares and Sharma, 2006).

Figure 3(d-f) shows particle deposition in the \( y \)-direction in the \( Re_b=83k \) flow. At the times considered the deposition ratio is low, as given in the figure. In all cases, the particles are ultimately seen to be deposited near the bottom of the wall at \( x^+=1930 \), with this trend more dominant with increasing particle size due gravity. Compared to the \( Re_b=250k \) flow, it is clear that the peak magnitude of the pdf is significantly higher for the lower Reynolds number due to deposition in this flow taking place at a faster rate than in the \( Re_b=250k \) case. However, it should be noted that, in terms of the deposition ratio in the \( y \)-direction, for all sizes of particle \( N_o/N \) is significantly higher in the \( Re_b=250k \) flow. This is likely associated with the increasing influence of the secondary flow on the deposition process with increasing Reynolds number. As for the \( Re_b=250k \) flow, the pdfs of the largest
particles in both the x- and y-directions have high values towards the duct side walls and floor, again indicating that the y preferentially deposit in the corners. Also, the smallest particles again tend to deposit near the centre of the floor. These findings are confirmed by the results of figure 3(d-f) which show an increasing tendency for deposition at the duct corners with particle size. Lastly, figure 3(g) and (h) gives results for deposition in the $Re_b=10k$ flow. It is seen that it takes a shorter time for the

**Figure 3.** Particle deposition in y-direction (a-c) $Re_b=250k$: (a) $50\mu m$ ($N_d/N=2%,5%,9%$); (b) $100\mu m$ ($2%,5%,9%$); (c) $500\mu m$ ($3%,5%,21%$) $t^*=83k$; - - -223k; - - -362k; (d-f) $Re_b=83k$: (d) $50\mu m$ ($0.04%,0.3%,0.4%$); (e) $100\mu m$ ($0.4%,2%,4%$); (f) $500\mu m$ ($0.5%,2.5%,7%$) $t^*=-11k$; - - -29k; - - -48k; (g),(h) $Re_b=10k$: (g) $50\mu m$ ($0.4%,0.9%$); and (h) $100\mu m$ ($0.2%,0.4%$) $t^*=-151$; - - -605.

**Figure 2.** Particle deposition in x-direction (a-c) $Re_b=250k$: (a) $50\mu m$ ($N_d/N=4%,8%,19%$); (b) $100\mu m$ (11%,27%,55%); (c) $500\mu m$ (17%,68%,92%) $t^*=-83k$; - - -223k; - - -362k; (d-f) $Re_b=83k$: (d) $50\mu m$ (2%,5%,12%); (e) $100\mu m$ (11%,30%,38%); (f) $500\mu m$ (86%,99%,100%) $t^*=-11k$; - - -29k; - - -48k; for (g-i) $Re_b=10k$: (g) $50\mu m$ (1%,17%); (h) $100\mu m$ (11%,69%) $t^*=-151$; - - -605; (i) $500\mu m$ (86%,97%,100%) $t^*=-302$; - - -454; - - -605. $N_d/N=$ (number deposited/total number) particles.
larger particles to deposit on the floor than it does for the $50\mu m$ particles due to the effect of gravity. In this flow the $50\mu m$ particles never deposited on the side walls, with all particles settling on the floor.

4. Conclusions
Particle deposition in turbulent duct flows has been investigated using large eddy simulation coupled to Lagrangian particle tracking. Deposition in the flows can be summarised as follows. In both the x- and y-directions, deposition is more variable with decreasing particle size. For the $Re_b=250k$ flow, the largest particles deposit in the duct corners, with this tendency increasing with particle size. In contrast, the smallest particles deposit near the centre of the floor of the duct. These findings are also generally true for the $Re_b=83k$ flow, although compared with the $Re_b=250k$ case, in the x-direction, deposition near the side walls happens at earlier times due to the effects of gravity, although there is less of a tendency for deposition near those walls. For the $Re_b=10k$ flow, the largest particles preferentially deposit near the centre of the duct floor at all times, in contrast with the higher Reynolds number flows, and these particles are also never observed to deposit near the side walls. These findings are in line with those of Winkler et al. (2006) and Phares and Sharma (2006).

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