The Influence of Gravity on Particle Collision and Agglomeration in Turbulent Channel Flows

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Abstract

The study described in this paper concerns the simulation of a particle-laden turbulent channel flow at high mass loadings, with and without the presence of gravity. Large eddy simulation (LES) is used to simulate the fluid phase, with solutions combined with a Lagrangian particle tracker to model the particle phase. Particle-particle interactions are detected using an algorithm based on a deterministic collision treatment (hard-sphere collision model), and particle agglomeration is based on the use of a particle restitution coefficient, energy balance and the sum of the van der Waals' force on each colliding particle. In order to establish the validity of the treatment, results are compared with those based on a DNS, with good agreement being found. Subsequent runs for colliding and agglomerating particles in a channel flow demonstrate that the rate of particle agglomeration peaks towards the channel walls due to increased particle concentrations and turbulence levels in these regions. Agglomeration is also greatly influenced by the presence of gravity, with this effect accentuated on the lower wall of the channel.

1 Introduction

The transportation of particulate materials is of importance in many engineering and industrial processes. Understanding the behaviour of such flows, in terms of how the particles are dispersed, can be used to improve flow assurance. Whilst it is important for particles to be transported at high concentrations in many industrial processes, it is also generally undesirable for particles to form agglomerates in such flows since agglomerates may deposit on solid surfaces within the flow, potentially leading to flow restrictions and ultimately pipeline blockage.

The agglomerate formation process is influenced by several factors such as particle velocity, collision frequency and the forces acting on the particles. Amongst those forces, the role of gravity in the formation process is significant and serves as the basis of this investigation.

To minimise cost, it is often necessary to employ a numerical simulation technique in the evaluation of such flows. Notable examples of such techniques are Reynolds-averaged Navier-Stokes (RANS) approaches, large eddy simulation (LES) and direct numerical simulation (DNS). LES is preferred in this study as it gives more accurate predictions when compared to those of the RANS method and, although DNS will inevitably yield more accurate predictions, its inability to accommodate high Reynolds number flows, as well as its high computational cost, makes LES the preferred choice for the present work. However, DNS continues to be a valuable technique in the prediction of multi-phase flows as it solves directly the instantaneous three-dimensional Navier-Stokes equations for the continuous phase without resorting to any modelling of turbulence, and hence is of significant value in improving our fundamental understanding of such flows.

Combining LES together with a Lagrangian particle tracking (LPT) technique improves the computational accuracy of turbulent flow predictions over those based on the RANS approach as the large scale turbulent motions arising in the flow are effectively resolved (with small eddies modelled), and particle motion within the flow is tracked using individual parcels of particles. Recent LES studies of particle-laden flows include those of Breuer and Alletto (2012), Mallouppas and van Wachem (2013), and Njobuenwu and Fairweather (2015). These authors studied the dynamics of particle-laden flows but only accounted for particle collision effects, neglecting agglomeration. Yao and Fairweather (2010, 2012) also studied particle re-suspension and deposition in a fully developed duct flow. Very few studies on particle agglomeration exist, although noteworthy examples are those of Afkhami et al. (2015) and Breuer and Almohammed (2015). However, the effect of gravity on agglomeration has not yet been considered. This study therefore investigates the effect of gravity on particle agglomeration in a four-way coupled system using LES and an energy-based particle interaction model (Breuer and Almohammed, 2015).

2 Numerical simulation

In this study, solution of the fluid dynamic equations was performed using the BOFFIN-LES code (Bini and Jones, 2008), with the sub-grid scale (SGS) stress arising from the top-hat filtering operation performed on the Navier-Stokes equations modelled using the Germano dynamic model. The fluid dynamic equations can be stated as:

$$\frac{\partial \bar{u}_j}{\partial x_j} = 0 \qquad (1)$$

$$\frac{\partial \bar{u}_i}{\partial t} + \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j} = -\frac{1}{\rho}\frac{\partial \bar{p}}{\partial x_i} - \frac{\partial}{\partial x_j}\left(\bar{\sigma}_{ij} + \tau_{ij}\right) + \bar{S}_{mom,i} \qquad (2)$$

where $\bar{\sigma}_{ij} = -2\nu\bar{s}_{ij}$ is the viscous stress, $\bar{s}_{ij} = \frac{1}{2}(\partial\bar{u}_i/\partial x_j + \partial\bar{u}_j/\partial x_i)$ represents the filtered strain-rate tensor, ν is the kinematic viscosity, $\tau_{ij} = \overline{u_i u_j} - \bar{u}_i\bar{u}_j$ represents the SGS stress (the SGS effect on the resolved motion), u_j is the velocity vector, x_j represents the spatial coordinate directions, t is time, p is pressure, and ρ the fluid density. The SGS tensor is computed using the dynamic version of the Smagorinsky model proposed by Piomelli and Liu (1995). In this model, the sub-grid scale viscosity is calculated as the product of the velocity scale and a filter width, $\Delta=(\Delta_x\Delta_y\Delta_z)^{1/3}$, while the stresses are computed as the product of the resolved strain tensor and the sub-grid scale velocity. A stochastic Markov model was also used to represent the influence of the unresolved fluid velocity fluctuations.

The number of grid nodes employed in computing the turbulent channel flow was 129×128×128 in the wall normal, spanwise and streamwise directions, respectively. Periodic boundary conditions were imposed in the streamwise and spanwise directions for both the fluid and the particles. At the channel walls, no-slip for the fluid phase and elastic collisions for the particle phase were assumed. The positions of the particles were randomly distributed initially within the flow, with their velocity equal to that of the surrounding fluid. The particle equation of motion was solved within an LPT code, with the fluid velocity field and the particle location computed using a fourth-order Runge-Kutta integration technique.

For the particles, the deterministic hard sphere collision model was used in the prediction of particle interactions within the fluid. In this model, the collision step is carried out in two stages. In stage 1, potential collision partners are identified by taking into account the smallest possible time steps within the flow, as collision during this time is only likely to happen between neighbouring particles. The likely particles are identified by the application of virtual cells across the channel domain. The inclusion virtual cells reduces the cost of the computation substantially from order $O(N_p^2)$ to $O(N_p)$. The cell size is dynamically adjusted to the smallest possible size (user dependent) to ensure that the number of particles in each cell is minimal. Particles within each cell are then tagged as having the best chance of collision. In stage 2, identified collision pairs are arranged according to their time of collision in ascending order. The particles are then repositioned to the point where collision occurs using the velocities at the time of impact. For more information on the collision model adopted, the reader is referred to the work carried out by Breuer and Alletto (2012).

For particle agglomeration, the model is based on the assumption that agglomeration will only occur if the relative kinetic energy of the particles post-collision is less than the energy required to overcome the van der Waals' forces of attraction between them. The expression for this is given in Eq. (3):

$$\frac{\left(\mathbf{v}_2^- - \mathbf{v}_1^-\right)^2 - \left[\left(\mathbf{v}_2^- - \mathbf{v}_1^-\right)\cdot\mathbf{n}_c\right]^2\left(1-e_n^2\right)}{|\left(\mathbf{v}_2^- - \mathbf{v}_1^-\right)\cdot\mathbf{n}_c|} \leq$$

$$\frac{H^*}{6\delta_0^{*2}}\left[\left(1-e_n^2\right)\frac{6}{\pi^2\rho_p^*\bar{\sigma}^*}\frac{d_{p,1}^{*3} + d_{p,2}^{*3}}{d_{p,1}^{*2}\,d_{p,2}^{*2}\left(d_{p,1}^* + d_{p,2}^*\right)}\right]^{1/2} \qquad (3)$$

where, in dimensionless terms, ρ_p^* is the particle density, d_p^* is the particle diameter, H^* is the Hamaker constant, $\bar{\sigma}^*$ is the yield pressure, u_b the bulk velocity and $2h$ the channel height. The superscript * represents dimensionless quantities. Further information on the agglomeration model adopted can be found in Breuer and Almohammed (2015).

The flow considered for all simulations used a shear Reynolds number $Re_\tau = u_\tau h/\nu = 300$ (based on the channel half height, h, the shear velocity, u_τ, the kinematic viscosity, $\nu = 10^{-6}$ m^2 s^{-1}, and the density $\rho = 10^3$ kg m^{-3}). The particles were assumed equal in size (diameter, $d_p = 125\mu m$, and density $\rho = 2710$ kg m^{-3}) with a volume fraction $\phi_v \sim O(10^{-3})$, thus giving a particle to fluid density ratio $\phi_p = 2.71$. The particle minimum contact distance was $\delta_0 = 3.36\times10^{-10}$ m, the mean yield stress $\sigma = 3.0\times10^8$ Pa, the Hamaker constant $H = 3.8\times10^{-20}$ J and the normal restitution coefficient $e_n = 0.4$. These values were used as they are representative of calcite (Ho and Sommerfeld, 2002; Tomas, 2007), a frequently used simulant in nuclear waste studies. The total number of particles present in the computational domain was 1,240,000 in all cases. Particle break-up was also assumed not to occur in order to completely isolate the influence of gravity on particle collision and agglomeration. All particles used, including agglomerates, were assumed spherical. Other assumptions were that particle-particle interaction due to collision is binary; only minimal particle deformation occurs post-collision; van der Waals' forces are solely responsible for particle adhesion after collision; and particle agglomeration is based on van der Waals' interactions and the pre-collision energy of the particles.

3 Results and discussion

In order to establish the accuracy of the LES-LPT method adopted, results were first validated against more accurate DNS-based solutions for the fluid phase (Marchioli et al., 2008). In Figure 1(a) and (b), the LES results for the single phase, despite a few discrepancies, show good overall agreement with those based on DNS, with the fluctuating velocities in particular being in close accord.

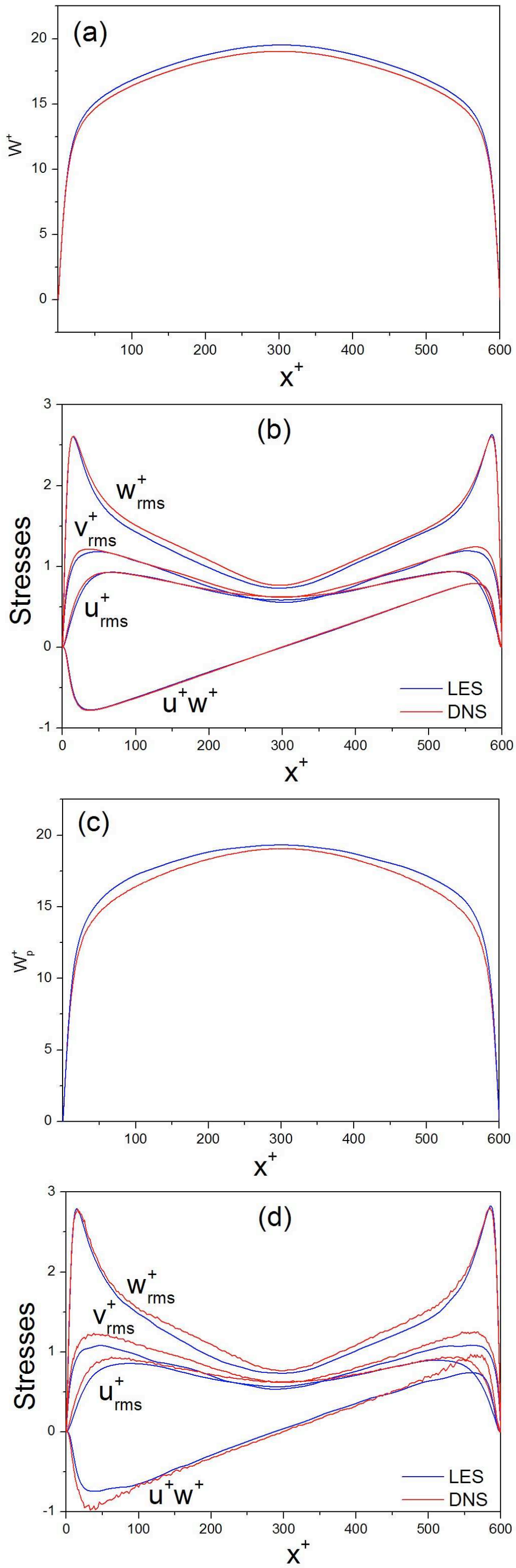

Figure 1: Comparison of LES and DNS-based predictions for: (a) single-phase mean streamwise velocity, (b) normal and shear stresses for the single phase, (c) particle phase mean streamwise velocity, and (d) particle phase normal and shear stresses.

The validation was also repeated for a dilute, one-way coupled particle-laden flow, the results of which are shown in Figure 1(c) and (d), with the predictions again showing a similar outcome in regards to the accuracy of the LES. Overall, therefore, the LES results showed good agreement with those based on DNS and hence can justifiably be used in this investigation.

Figure 2(a) compares the collision count, N_{col}, up to a simulation time of $t^+ = 1000$ and the number of agglomerates, N_{agg}, formed as a result of those collisions (x^+ is the wall distance). Clearly, not all collisions result in the formation of agglomerates, and there are far more collisions in the flow when compared to those that result in agglomeration. However, the simulations with gravity show a much higher rate of collision and agglomeration (locally) when compared to the zero gravity case. It is observed for both cases that there is a sharp increase in the rate of collision and agglomeration during the initial stages of the simulation, up to time $t^+ \approx 10$, after which the simulations show a decreasing rate of collision and agglomerate formation. When gravity is included, this increase is much greater, with the rate of collision and agglomeration continuing to increase with time and to be significantly greater than for the no gravity case.

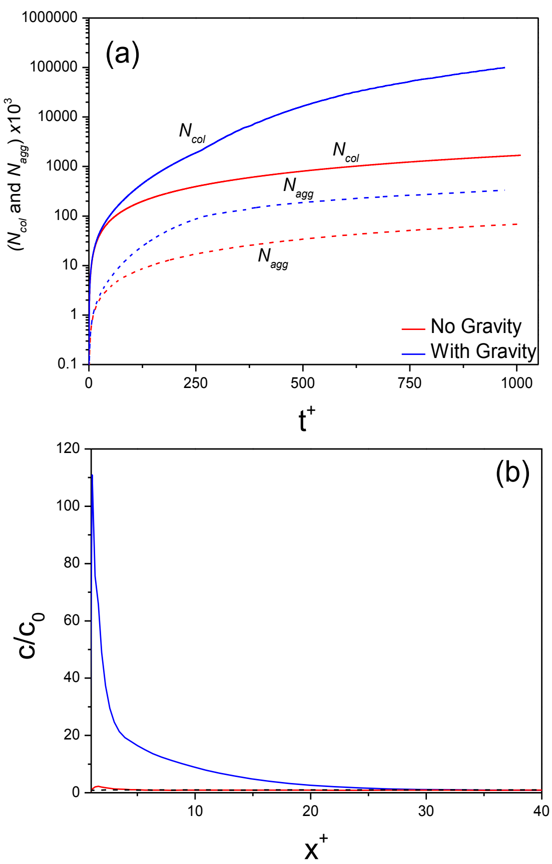

Figure 2: (a) Total number of collisions and agglomerates formed with time, and (b) particle concentration profile across the channel.

Further analysis, shown in Figure 2(b), demonstrates that the above findings are due to the influence of gravity, which promotes particle migration towards the lower wall of the channel into areas of high turbulence. This in turn increases the particle concentration in areas near the lower wall, with increased turbulence levels promoting both collision and agglomeration.

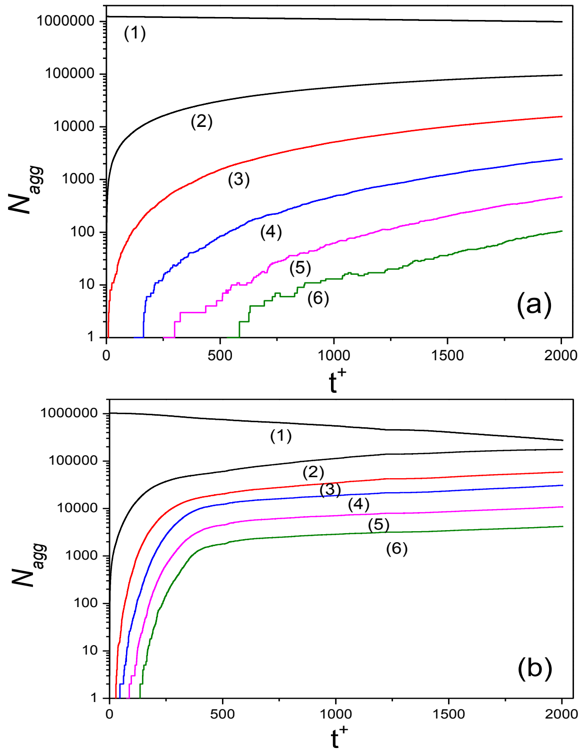

Figure 3: Agglomerate formation with time across the channel: (a) without gravity and (b) with gravity. Line numbers: single (1), double (2), triple (3), quadruple (4), quintuple (5), sextuple (6).

Figure 3 further illustrates the influence of gravity on the formation of agglomerates. In Figure 3(a), the rate of depletion of single particles during the agglomeration process, and the corresponding evolution of multi-sized particles, up to a simulation time of t^+ = 2000 is shown. At the start of the simulation, the results indicate a sharp increase in the number of double and triple particles formed at short times ($t^+ <$ 10), which can be attributed to the influence of the initial conditions in the flow. However, after an increased processing time ($t^+ \approx$ 100), the rate of formation of multi-sized particles reduces to a more steady state as interactions with the turbulent flow structures increase causing a reduction in localized particle interactions. Figure 2(b) demonstrates that the inclusion of gravity enhances the rate of depletion of the single particles and the rate of formation of secondary particles (double, triple, quadruple, etc.). Over the specified simulation time, it is observed that more of the single particles form agglomerates for the flow under gravitational influence, with an initial sharp increase in their formation that eventually reaches a pseudo-steady state by $t^+ \approx 350$. This contrasts with the no gravity case where the number of agglomerates continues to increase more significantly with time, albeit at lower levels for each multiple particle type.

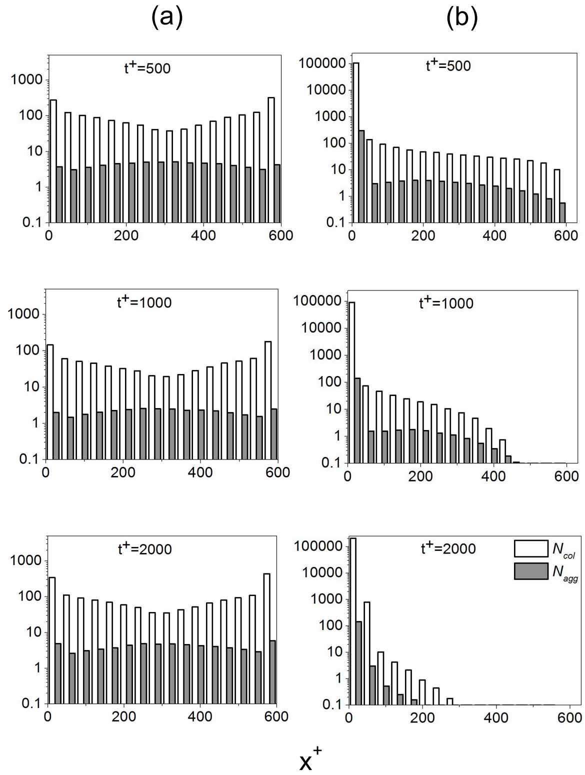

Figure 4: Distribution of particle collisions and agglomerates across the channel for (a) no gravity and (b) gravity cases (ordinate is N_{col} and N_{agg} $\times 10^3$).

Figure 4 provides information regarding the particle distribution across the channel and the locations where collisions occur and agglomerates are formed. The cross-stream domain is divided into 16 equally spaced slabs, with combined particle statistics given within each of these regions. Slab 1 through 16 represents movement from the lower to the upper wall of the channel. The results were derived at mean time values of t^+ = 500, 1000 and 2000, averaged over $t^+ \pm$ 500 at each time point to provide a sufficiently large sample. For all cases with zero gravity, Figure 4(a), the number of collisions is roughly symmetric, with maxima in the two near-wall regions. The number of agglomerates formed in this case is small, although peaks are seen close to the walls where turbulence levels are high. It is also observed that the formation of agglomerates for the zero gravity case additionally gives a maximum within the bulk of the flow where turbulence levels are less significant. It is important to note that when particles collide within this less turbulent region, their combined elastic energy after dissipation is in most cases too low to overcome the attractive forces existing between them and therefore particle agglomeration is encouraged.

For the with gravity case, Figure 4(b), the trend is noticeably different, with the number of collisions and agglomerates in the upper wall region decreasing over time as particles deposit in the flow and increase their number close to the lower wall. From the results at t^+ = 500, there is a gradual migration of the particles towards the lower region of the channel, with the agglomerates reasonably distributed across each slab. By t^+ = 1000, more of the particles have migrated towards the lower wall, with almost no collisions or agglomeration now occurring in the upper regions of the flow. By t^+ = 2000, it is clear that there are no particles left in the upper half of the channel, with all the particles having now migrated towards the lower wall, leading to far more collisions and agglomeration in the region. As already noted, therefore, gravity leads, with time, to increased concentrations of particles in the lower wall region where turbulence levels are high and collision and agglomeration are promoted. It is noteworthy that the gravitational influence on particle migration from the upper to the lower wall region is clearly very significant for the particles considered in this study, with a rapid increase in particle concentration near the lower wall with time, and significantly larger numbers of collisions and agglomerates formed relative to the no gravity case. Beyond t^+ = 2000, particles under the influence of gravity were found to deposit out from the flow altogether.

Lastly, the influence of the particles, with and without the influence of gravity, on the mean flow velocity, and the normal and shear stresses, is considered in Figure 5 through comparisons with the fluid-only solution. For both cases, the impact of the presence of particles, which are four-way coupled with the flow, on the fluid mean velocity is slight, although some effect of gravity on the mean velocity is observed towards the lower wall and in the central region of the channel. Overall, the differences between the with and zero gravity cases, Figure 5(a), are negligible, although more significant modifications of the turbulence field can be noted in Figure 5(b). In particular, for the with gravity case, the normal and shear stresses are significantly enhanced by the high concentration of particles in the lower wall region in all three co-ordinate directions, and attenuated slightly towards the upper wall. Although true for all co-ordinate directions, the impact is more pronounced for the fluctuating velocity in the streamwise direction. For the zero gravity case, the stress in the streamwise direction is only slightly enhanced towards both wall regions, and slightly reduced for those in the other co-ordinate directions. The effect on the shear stress is negligible. Overall, therefore, and at the given simulation time of t^+ = 2000, particle collision, agglomeration and deposition in the with gravity case significantly increases the particle concentration near the lower wall with an associated increasing influence on the fluid flow field.

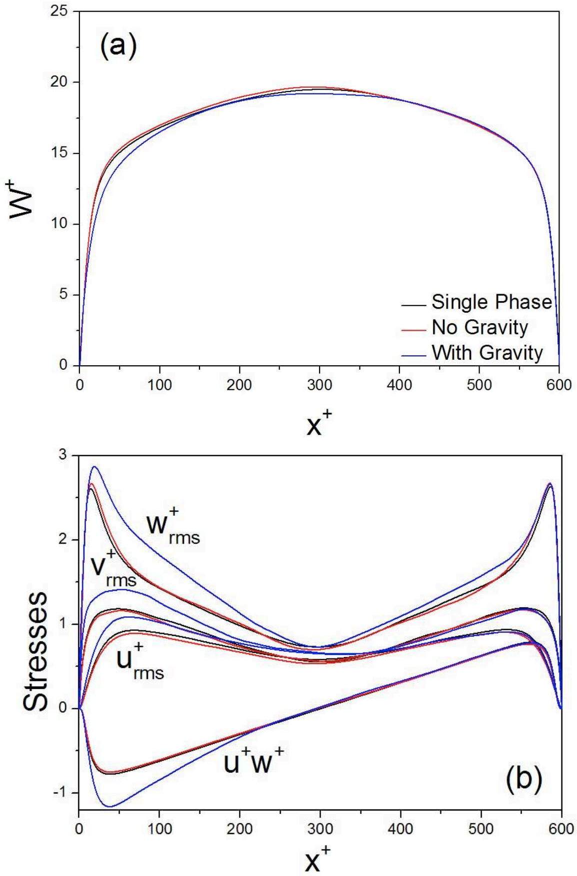

Figure 5: (a) Fluid streamwise mean velocity and (b) normal and shear stresses for the single phase.

4 Conclusions

Large eddy simulation coupled with a Lagrangian particle tracking technique has been employed to predict the influence of gravity on particle interaction and agglomeration at moderate turbulence levels in a channel flow. Results derived for cases with and without the influence of gravity show that particle interaction and agglomeration is strongly influenced by gravity, which promotes particle migration towards the lower wall of the channel into areas of high turbulence. This in turn increases the particle concentration in areas near the lower wall, with increased turbulence levels promoting collision and agglomeration. The influence of gravity therefore promotes particle deposition, over and above what would be expected from one-way coupled simulations, though the enhancing mechanism of particle agglomeration. Such effects have significant practical implications in many industrial processes.

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