PARTICLE VOLUME FRACTION EFFECTS IN SIMULATIONS OF TURBULENT CHANNEL FLOWS

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Abstract

Direct numerical simulation and a Lagrangian particle tracking routine are used to simulate multiphase particle-laden flows through a channel at a shear Reynolds number of 300. The overall model is used to simulate 300k solid particles with a diameter of 100 μm at different levels of coupling between the particles and the flow field. In an attempt to reduce computational cost, a stochastic inter-particle collision model is implemented, which produces promising results. However, when the particle size, and hence volume fraction, is increased to 200 μm the predicted particle normal stresses no longer agree with results based on a fully deterministic collision approach.

To resolve this a second stochastic method is implemented based on a direct simulation Monte Carlo approach which generates probable collision events from pairs of nearby particles. The predictions based on this method are found to be satisfactory for both sizes of particle, and to be in good agreement with results based on the fully deterministic approach.

1 Introduction

Accurately simulating particle-laden flows is of fundamental importance to many industries that, as part of their operations, are required to transport multi-phase mixtures, including waste. This includes industries in the chemical, pharmaceutical, agriculture and minerals processing sectors, and of particular interest here, the nuclear industry. Without proper optimisation, these processes can be inefficient and lead to potentially hazardous blockages or depositions of, in some cases, corrosive or radioactive substances which in turn may require expensive and sometimes hazardous maintenance procedures to resolve.

Under complex turbulent flow conditions, it is difficult, if not impossible, to exactly predict the dynamic interactions between a fluid and the particles within it using conventional mathematical modelling approaches. Experimentation also often produces inconsistent results due to the difficulty in repeating initial conditions. Hence this work turns to computer-based modelling methods. Direct numerical simulation (DNS) is an approach which resolves the entire flow, over all length and time scales, and all of the turbulence effects within it. This, when coupled to a method for predicting the behaviour of individual particles within the dispersed phase, produces comprehensive information about the properties of a multiphase flow.

The disadvantage of DNS is of course its high computational cost, particularly when compared to simpler prediction methods such as Reynolds-averaged Navier-Stokes (RANS) approaches. However, by using DNS to assess the behaviour of particles within a multi-phase flow it is possible to establish useful benchmarks which can be used to verify the output of less accurate methods such as RANS and large eddy simulation (LES). Additionally, by increasing the level of coupling between the continuous and dispersed phases, the DNS-Lagrangian particle tracking approach can be used to accurately assess the impact of the particles on the flow field, and again provide benchmark solutions of value in improving the accuracy of RANS and LES approaches.

In recent years, such flows have been simulated by, for example, Squires and Eaton (1990), Sundaram and Collins (1999), and Li et al (2001). Important findings include the fact that turbulence intensities grow more anisotropic as the particle mass loading is increased. Work by Vremen et al (2009) and, more recently, by Rupp et al (2017) also qualitatively describe the way particles affect the continuous phase at high concentrations. However, with regard to the effects of varying particle volume fraction on the continuous phase, the literature is lacking.

Furthermore, running deterministic simulations at high particle concentrations requires significant computational resources, thus the present work focuses not only on the effect of particle volume fraction, but also on methodologies for making high volume fraction flows less laborious to simulate by using stochastic alternatives to fully deterministic approaches to produce results of the same level of accuracy over shorter timescales.

2 Methodology

The fluid flow is simulated using a spectral element method, a hybrid of the finite-element method and the spectral method, which was developed by Patera (1984). The fluid domain is divided into elements with a resolution finer than 15 times the Kolmogorov scale, which Moser and Moin (1984) have shown to be the minimum requirement in performing direct numerical simulations.

$$\frac{\delta \boldsymbol{u}^*}{\delta t^*} + (\boldsymbol{u}^* \cdot \nabla)\boldsymbol{u}^* = -\nabla p^* + \frac{1}{Re}\nabla \cdot \tau^* + f_i \quad (1)$$

$$\nabla . \boldsymbol{u}^* = 0 \quad (2)$$

Equations (1) and (2) are the non-dimensional, incompressible Navier-Stokes and continuity equations solved, where $\boldsymbol{u}^*$ is the fluid velocity vector, which has been non-dimensionalised using the bulk velocity U_B, and t^* is the non-dimensionalised time tU_B/δ, where δ is half the height of the channel. p^* is a non-dimensionalised pressure term equal to $p/\rho U_B^2$, where ρ is the density of the continuous phase. Re is the bulk Reynolds number given by $\delta U_B/\nu$, and τ^* is the non-dimensionalised deviatoric stress tensor given by $\tau^* = (\nabla \boldsymbol{u}^* + \nabla \boldsymbol{u}^{*\tau})$. f_i is an arbitrary forcing term that is only applied to flows with multiple phases. The code used to simulate the fluid flow was Nek5000, an efficient DNS code developed by Fischer et al. (2008).

The fluid flow equations were solved for a turbulent flow in a channel with dimensions 12δ × 2δ × 6δ at a bulk flow Reynolds number of 4900, which translates to a shear Reynolds number of 300. The channel had periodic boundary conditions in the streamwise and spanwise directions, making its size arbitrary in those directions, with the channel wall having a significant effect on the flow. The computational domain was divided into 32 × 32 × 32 elements consisting of 8 × 8 × 8 nodes each, giving a total of 16.8M nodes.

The multi-phase flows simulated considered two different sizes of particles using a versatile Lagrangian particle tracking code which synchronises with the Eulerian fluid flow model, time-step for time-step.

$$\frac{\partial \boldsymbol{x_P^*}}{\partial t^*} = \boldsymbol{u_P^*} \quad (3)$$

$$\frac{\partial \boldsymbol{u_P^*}}{\partial t^*} = \underbrace{\frac{3C_D|\mathbf{u_S^*}|}{4d_p^*\rho_P^*}\mathbf{u_S^*}}_{Drag} + \underbrace{\mathbf{g}^*(1-\rho^*)}_{Gravity} \underbrace{\frac{3}{4}\frac{C_L}{\rho_P^*}(\mathbf{u_S^*} \times \boldsymbol{\omega}_F^*)}_{Lift} + \underbrace{\frac{1}{2\rho_P^*}\frac{D'\mathbf{u_F^*}}{Dt^*}}_{Virtual\ Mass} + \underbrace{\frac{1}{\rho_P^*}\frac{D\mathbf{u_F^*}}{Dt^*}}_{Pressure\ Gradient} \quad (4)$$

The tracking code solves Equations (3) and (4) for $\partial x_P^*/\partial t^*$, the change in non-dimensional position over non-dimensional time, for each particle using the fourth order Runge-Kutta method, as described in Suli and Mayers (2003). d_p^*, ρ_P^* and ρ^* are the non-dimensional particle diameter, density and fluid density, respectively, and $\boldsymbol{u_s^*}$, $\boldsymbol{u_F^*}$ and $\boldsymbol{\omega}_F^*$ are the slip velocity, fluid velocity and vorticity, with C_D, C_L and $\mathbf{g}^*$ being the coefficients of drag, lift and gravity.

For two-way coupling between the particles and the fluid, and above, the effect of the particles on the fluid must be considered. A term is added to Equation (5) to account for this:

$$f_C = \frac{1}{V}\sum(P=1)^N F_P \quad (5)$$

Here, V is the volume of a computational cell, N is the number of particles it contains, and F_P is the force exerted on any particle P. In order to gauge the effect of neglecting higher levels of coupling, the 100 μm and 200 μm glass particles were run at three levels of coupling: one-way, two-way and four-way. In four-way coupling, the fluid-particle, particle-fluid, and particle-particle interactions are all taken into consideration.

Inter-particle collisions were simulated by checking the radius of a particle and comparing it to each potential collision partner in a region of the flow, extrapolating backwards to find the time of collision and changing the particle velocity and position accordingly. In order to limit computer run times, the flow was divided into small segments, and only those particles in the same segment of the flow were considered for collision. However, even using that compromise, the number of operations rises with the square of the number of particles.

A method of decreasing the computational expense present in monitoring particle-particle interactions is to use a stochastic method which forgoes the monitoring of inter-particle collisions in favour of treating them as probabilistic events, in this case using kinetic theory to predict the likelihood of such a collision occurring.

Sommerfeld (2001) demonstrates a method whereby for each particle in a region, a fictional particle is generated using the averaged statistics of the particles in that same region. This particles is given a fluctuating velocity $u'_{fict,i}$, Equation (6), which accounts partially for the velocity of the real particle, $u'_{real,i}$, and partially for the RMS velocity of the regional particles, $\sigma_{p,i}$. The ratio between these is dependent on a Stokes correlation function *R(St)* given in Equation (7), and a Gaussian random number ξ:

$$u'_{fict,i} = R(St)u'_{real,i} + \sigma_{p,i}\sqrt{1-R(St)^2}\xi \quad (6)$$

$$R(St) = \exp(-0.55 \times St^{0.4}) \quad (7)$$

$$P_{coll} = f_c \Delta t = \frac{\pi}{4}\left(2D_\mathrm{p}\right)^2 \left|\overrightarrow{u_{\mathrm{p},i}} - \overrightarrow{u_{\mathrm{p},j}}\right| n_\mathrm{p} \Delta t \quad (8)$$

The probability of collision is then given by Equation (8), based on the instantaneous relative velocity $|\overrightarrow{u_{p,i}} - \overrightarrow{u_{p,j}}|$ between the fictional and the real particles, the number density n_p and the particle diameter D_p.

After the results from this first method were obtained and found to be lacking in certain respects, a second stochastic approach was also investigated to serve as an alternative and for comparison purposes. This was the direct simulation Monte Carlo (DSMC) method described by Pawar et al (2014). Like the previous method, the DSMC stochastic method uses kinetic theory to determine the probability of a collision occurring, but instead of generating a fictional collider for each particle, it selects a particle within a certain range of the particle of interest and initiates a collision between them if a randomly generated number falls below the probability of said particles' colliding.

Since the particles being probabilistically collided are real particles within the flow, it avoids making the same kind of assumptions about velocity fluctuations that are present within the method that uses fictional particles. In the DSMC approach, part of the described method is the use of a spherical searching scope which ensures that each particle has a random collider selected from the region in which it is centred. This is used to prevent the lattice artefacts produced by particles failing to interact across boundaries such as those of the segments used in this study. However, such a procedure conflicts with the intent of this study which is to minimise the number of computational operations performed per particle.

A second approach, therefore, is to use Equation (8), since kinetic theory was used in both stochastic approaches to generate the probability of collision between randomly selected particle pairs within the same segment. Any lattice artefacts produced will therefore be consistent between the deterministic four-way coupled approach, the stochastic approach, and the stochastic-DSMC approach.

3 Results and discussion

For all the simulations the mean streamwise fluid velocity, as well as the mean streamwise particle velocity, remained consistent and essentially equal, whatever the level of coupling. Mean velocity predictions are therefore omitted from what follows in the interests of brevity.

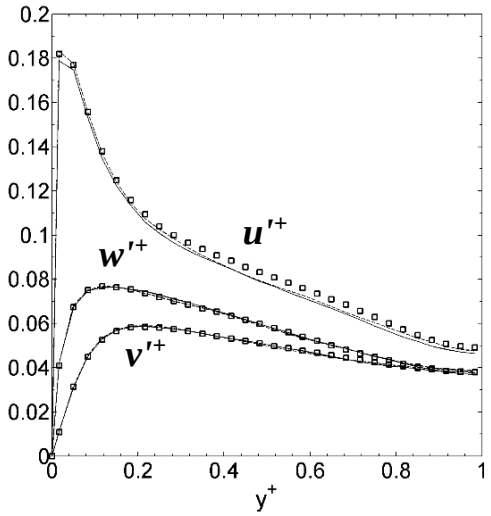

Figure 1: Normal particle stresses for a channel flow with 300k 100 μm particles (one-way coupled – solid line, two-way coupled – dashed line, four-way coupled – □).

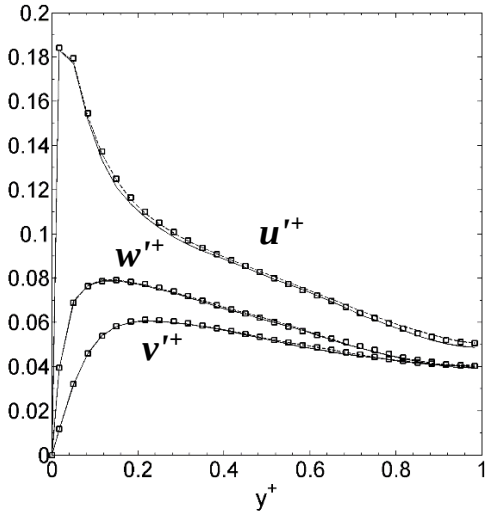

Figure 2: Normal particle stresses for a channel flow with 300k 200 μm particles (key as Figure 1).

Figures 1 and 2 show the particle normal stresses for two different sizes of particles at three different levels of coupling. The overall finding is that increasing the level of coupling has a negligible effect, especially for the larger class of particles. However, for both cases the effect is most notable upon the streamwise particle velocity fluctuations.

The greatest difference is in the streamwise velocity fluctuations of the 100 μm particles, particularly between $0.2 \leq y^+ \leq 0.7$, where the four-way coupled particles show a larger streamwise velocity fluctuation than for the other levels of coupling. This is due to the smaller and therefore less inertial particles rapidly changing their velocity due to collisions, the majority of which happen in the noted region. Interestingly for the

200 μm particles in that same region, the fluctuating velocities are approximately equal whatever the coupling level. The conclusion which can be drawn from this is that just as the low inertia particles experience large changes in velocity that drive increases in its normal stress, the high inertia particles experience fewer collisions with the particles' inertia resulting in less impact of those collisions on the particle velocity.

Figure 3 compares results from the stochastic model for the 100 μm particles with those from the deterministic four-way coupled approach. Though it is clear that the velocity fluctuations are slightly more energetic for the stochastic approach, again with the largest effect in the $0.2 \leq y^+ \leq 0.7$ region, overall the differences between the two approaches are very small.

The same cannot be said for the 200 μm particles, results for which are given in Figure 4. While the mean streamwise velocity was unaffected whatever the method, the increased size of the particles greatly magnifies the slight differences in velocity fluctuations observed for the smaller particles. Certainly differences between the fluid and particle stresses are now apparent, due to the increased particle inertia. However, significant differences now occur between the deterministic and stochastic approaches, and these grow as the centre of the channel is approached.

The stochastic DSMC results shown in Figures 5 and 6 demonstrate a strong agreement with the deterministic predictions for both sizes of particle. The results for the 100 μm particles are in slightly poorer agreement with the deterministic approach than is the case for the non-DSMC stochastic method, with the particles and the fluid displaying smaller streamwise velocity fluctuations than the deterministic predictions in this case. However, the accuracy of the predictions does not drop nearly so dramatically as the particles increase in size. In fact, the DSMC seems to be producing a small underestimation of the particle velocity fluctuations when compared to the deterministic approach, although this is generally small enough to be ignored.

By plotting the particle number density function across the channel the behaviour of the particles can be analysed in more detail. The results are shown in Figures 7 and 8. Immediately a difference can be seen between the distributions of the 100 μm and the 200 μm particles. Both distributions are seen to peak close to the wall, in regions of the flow where the deviations between results shown in Figure 4 are at their smallest.

For all methods of collision, the 100 μm particles have a particle concentration that shows a general decrease, past the initial peak at the wall, as the centre of the flow is approached. The 200 μm particles, in contrast, show a sharp drop in concentration moving away from the peak near the wall, with this concentration subsequently increasing gradually as the centre of the channel is approached.

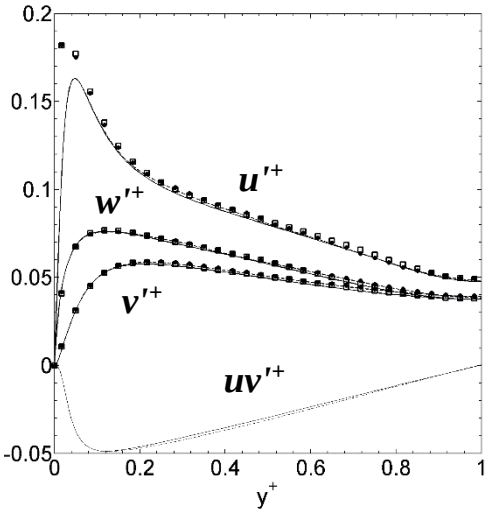

Figure 3: Fluid and particle normal and shear stresses for a channel flow with 300k 100 μm particles (fluid: deterministic – solid line, stochastic – dashed line; particles: deterministic – □, stochastic – ●).

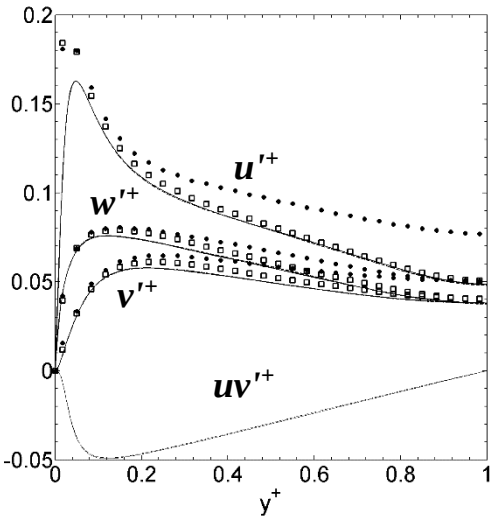

Figure 4: Fluid and particle normal and shear stresses for a channel flow with 300k 200 μm particles (key as Figure 3).

The reasons for these distributions are clear. The wall region of a channel flow has different properties to the central region, with the flow velocities reduced and the pressure lower. Particles drift into this region due to turbophoretic effects, which result in increased particle concentrations near the wall due to the inhomogeneity in the wall-normal velocity fluctuations, and tend to remain there. For more details about wall region effects see Mortimer et al (2017).

For the larger particles, this effect is noticeably smaller, since their greater inertia tends to carry them through the wall region, where they rebound off the wall, or another particle, back into the bulk of the flow. More 200 μm particles are present in the centre of the flow, with the 100 μm particles showing little difference across the majority of the flow. The presence of an increasing number of 200 μm particles as the channel centre is approached ties in with the over-prediction of fluctuating velocities by the stochastic model in Figure 4.

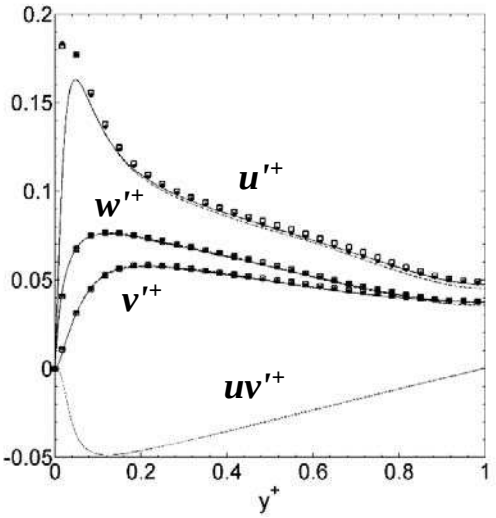

Figure 5: Fluid and particle normal and shear stresses for a channel flow with 300k 100 μm particles (fluid: deterministic – solid line, stochastic DSMC – dashed line; particles: deterministic – □, stochastic DSMC – ●).

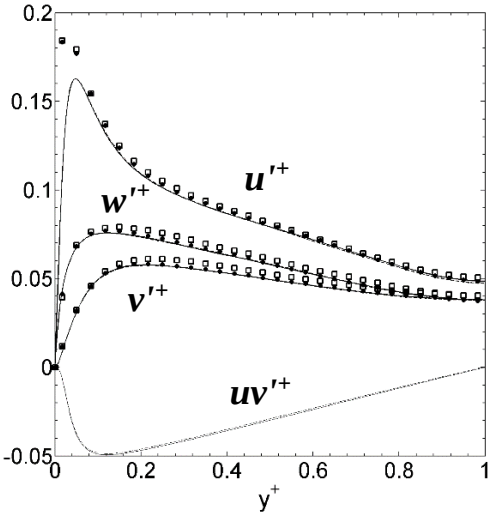

Figure 6: Fluid and particle normal and shear stresses for a channel flow with 300k 200 μm particles (key as Figure 5).

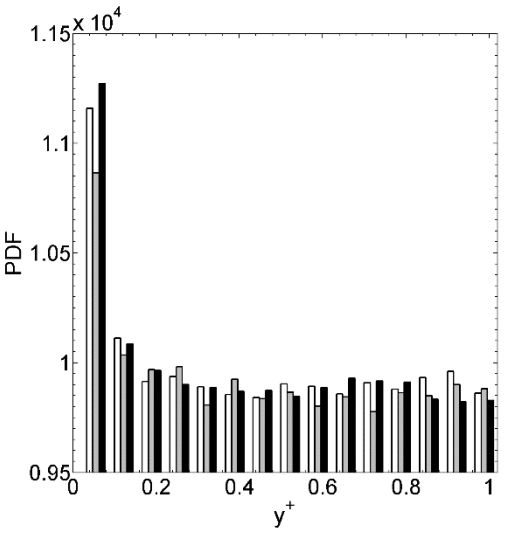

Figure 7: Particle number density function for a channel flow with 300k 100 μm particles (deterministic – white, stochastic – grey, stochastic DSMC – black).

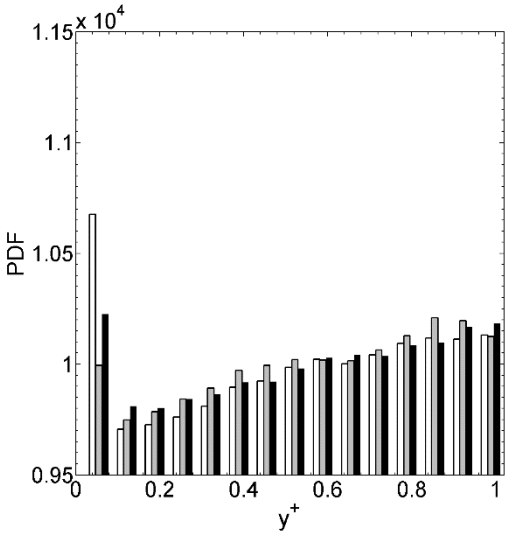

Figure 8: Particle number density function for a channel flow with 300k 200 μm particles (key as Figure 7).

With more, and larger, particles present towards the centre of the flow in this case, more particle collisions occur in this region. This increased number of collisions leads to the exaggeration in the predictions of the stochastic model being magnified, an effect that is less severe for the DSMC model because of its fewer assumptions. Another trend in the results of Figure 8 is the higher concentration of DSMC particles near the wall when compared to the stochastic approach predictions, although both stochastic approaches underestimate the deterministic results, which could imply a decreased accuracy in the former methods in this region.

4 Conclusions

This work has investigated the effects of particle volume fraction on the properties of multiphase flows in a channel at a shear Reynolds number of 300, achieved using two different sizes of particle.

By using different levels of coupling between the particles and the fluid flow, it has been possible to demonstrate the magnitude of different effects produced by changing the size of the particles. For instance, that smaller particles show more influence of the inclusion of inter-particle collisions than larger ones, or rather, are more dependent on a higher level of coupling for the purposes of predictive accuracy.

A comparison has been made between different methods of predicting inter-particle collisions in order to determine if a desired reduction in computational processing requirements necessarily leads to a reduction in predictive accuracy. For 100 μm particles, the stochastic methods considered demonstrated results that matched predictions of a deterministic approach. However, in the case of 200 μm particles, assumptions made regarding fictional particles caused an over-prediction of particle velocity fluctuations, particularly towards the centre of the flow where more collisions occur.

Analysis of the particle number distribution shows a predisposition, for both sizes of particle, to accumulate close to the channel walls. However, the larger particles also show a similar disposition to accumulate at the centre of the channel, providing an additional reason for the over-prediction of particle normal stresses in this region, beyond those due to the increased collision frequency due to particle size.

Use of a direct simulation Monte Carlo-based stochastic approach resulted in good agreement with deterministic results for both particle sizes. Further work will consider testing of these effects in a lower density fluid, and for larger particles, situations which are likely to try the seemingly high effectiveness of the DSMC method.

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