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THE APPLICABILITY OF THE EULERIAN-EULERIAN CFD APPROACH USING GRANULAR KINETIC THEORY TO PREDICT PARTICLE SETTLING AND MIGRATION IN VISCOPLASTIC FLUIDS

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Granular kinetic theory (GKT), while developed for fluidized beds typically consisting of gaseous and particulate phases has also found success in modelling Newtonian fluid and coarse solids slurry flows in tanks and pipelines. However, many mineral processing slurries are treated as a coarse particle fraction suspended within a non-Newtonian viscoplastic carrier fluid. Three model scenarios are considered in this study to evaluate the applicability of the GKT approach in an Eulerian-Eulerian framework for viscoplastic fluids: basic hindered particle settling within a quiescent fluid, neutrally buoyant particle shear migration, and particle settling under simple Couette shear. The study considers the three scenarios for both Newtonian and viscoplastic fluids and compares them to experimental results found in the literature. Based on this study, granular kinetic theory appears suitable in predicting Newtonian hindered settling, but unable to predict the particle migration due only to shear of the neutrally buoyant particles. The predictions for particle settling under Couette shear in viscoplastic fluids are promising considering the limited current understanding of the phenomenon, but model adaptations are required to better predict the behaviour.

KEY WORDS: CFD, viscoplastic, granular kinetic theory, Eulerian-Eulerian, shear migration, hindered settling

1. INTRODUCTION

Computational methods are more frequently being utilized to better understand slurry flow behavior. The Eulerian-Eulerian method is commonly employed as it typically provides sufficient accuracy while maintaining a high level of computational efficiency. The Eulerian-Eulerian particle framework in the CFD package Ansys Fluent 15.0 (2014) utilizes granular particle closure models to determine the particle volume fraction behavior.

The granular particle models, based on granular kinetic theory (GKT), were originally developed for gas-solids flows such as fluidized beds. However, they have been found to be applicable in predicting the concentration and velocity gradients within slurry pipeline flows of water and coarse solids (Kaushal et al., 2012); as well as sedimentation within mixing tanks (Wadnerkar et al., 2012). These comparisons have been limited to relatively large (tens of μm to mm scale) particles and Newtonian (water) carrier fluids.

The objective of this study is to complete a high level investigation of the granular particle method to gauge its ability to predict particle motion in Newtonian and non-Newtonian viscoplastic fluid. The authors have attempted to replicate experimental results provided in the literature for three basic flow scenarios: hindered particle settling, particle migration due purely to fluid shear, and sheared particle settling.

1.1. MODEL BACKGROUND

The Eulerian-Eulerian granular model in Ansys Fluent 15.0 is developed based on granular kinetic theory (GKT). The fundamental equations for the model are summarized in Wadnerkar et al. (2012) and therefore are not discussed here.The theory is based on the concept of granular temperature, a quantification of the random particle motion within the finite volume and defined as one third the mean square particle velocity Gidaspow (1994):

$$\Theta = \frac{1}{3}\sqrt{u_s : u_s}. \quad (1)$$

The granular temperature is proportional to the kinetic energy contained in the particle phase, and is used to determine the conservation and transfer of energy and momentum between the solid and fluid phases. Various options are available in Fluent for the different components comprising the GKT model. Table 1 summarizes the parameters used in this analysis. This selection is based on the findings from Yang (2009) and Kaushal (2012) along with recommendations from the Fluent user's manual (2012).

Table 1. Granular Kinetic Theory (GKT) Model Parameters

Parameter	**Model**
Granular Viscosity	Gidaspow
Granular bulk viscosity	None
Frictional viscosity	None (default)
Granular temperature	Algebraic (default)
Solids pressure	Lun et al (default)
Radial Distribution	Lun et al (default)
Elasticity Modulus	Derived (default)
Packing limit	0.61

2. EVALUATION CASES

The GTK model evaluation considers three basic scenarios:Quasi-static settling of negatively buoyant (heavy) particles, Couette shear migration of neutrally buoyant particles, and settling of negatively buoyant particles under Couette shear flow. The evaluation cases compare the results obtained using the GTK CFD modelling to the experimental results provided in various literature results for each representative case. Table 2 summarizes the comparison cases.

Mesh convergence studies on the initial case geometries indicated the overall average velocity and concentration profiles did not vary significantly with variation in mesh size. However, a finer mesh results in better resolution of the localized concentration and velocity variations. The selected meshes sizes for each case had sufficient resolution to provide adequate comparison to the published results. The GKT CFD analyses utilized a phase coupled SIMPLE pressure-velocity scheme, least squares cell based gradients, and second order upwind numerical methods for momentum and time. The absolute residual's convergence was 10^{-6} for continuity and 10^{-5} for the remaining parameters.

Table 2. Analysis Cases

Case	(A) Newtonian	(B) Non-Newtonian
1) Quasi-Static Settling	Richardson & Zaki (1954) Garside & Al-Dibouni (1977)	Critical yield stress criterion from Chhabra (2008)
2) Shear Particle Migration	Philips et al. (1991) geometry and results	Rao et al. (2002) geometry and results
3) Shear settling of Particles	No evaluation in this study	Ovarlez et al. (2012) geometry and results

2.1 CASE 1A – QUASI-STATIC SETTLING – NEWTONIAN FLUID

The first evaluation case considers the basic scenario of particle settling within a quasi-static fluid. For this evaluation, the hindered settling velocities from the CFD results using GTK are compared to the well-known Richardson and Zaki (1954) relationship:

$$V_{HS} = V_{ts}(1-\alpha_s)^n, \tag{2}$$

where n is a function of the particle Reynolds number, summarized in Table 3. V_{ts} is the stokes settling velocity as determined using the particle drag coefficient correlation of Cheng (2009):

$$C_D = \frac{432}{d^{*3}}\left(1+0.022d^{*3}\right)^{0.54} + 0.47\left[1-exp\left(-0.15d^{*0.45}\right)\right] \tag{3}$$

where

$$d^* = d\left[\frac{\rho_l g(\rho_s-\rho_l)}{\mu_l^2}\right]^{1/3},\ V_{ts}{}^* = V_{ts}\left[\frac{\mu_l g(\rho_s-\rho_l)}{\rho_l{}^2}\right]^{-1/3}, \text{and } V_{ts}^* = \sqrt{\frac{4d^*}{3C_D}} \tag{4}$$

Table 3. Hindered settling coefficient

$Re_{p=}$	n
$Re_p < 0.2$	$n = 4.6$
$0.2 < Re_p \leq 1.0$	$n = 4.4\ Re_p^{-0.03}$
$1.0 < Re_p \leq 500$	$n = 4.4\ Re_p^{-0.1}$
$Re_p > 500$	$n = 2.4$

Garside and Al-Dibouni (1977) developed an improved relationship, provided in equation (5), relating the Richardson and Zaki exponent to the particle Reynolds number. The computational results are compared to the hindered settling velocity predictions using both empirical relationships for n.

$$\frac{5.1-n}{n-2.7} = 0.1{Re_p}^{0.9}\ . \tag{5}$$

Model Geometry and Material Properties

The authors modelled a 45 mm diameter by 300 mm tall static settling cylinder using hexahedral elements for the study. The walls were treated as no-slip for both the fluid and solid phase following findings of Balakin et al., 2010. The evaluation considered either 100 micron or 1000 micron monosized spherical particles with solids density of 2.65 g/cm^3 and solids volume fractions from 5% to 50%. The fluid fraction was water with a density of 0.998 g/cm^3 and 1.03 mPa.s dynamic viscosity.

Results and Discussion

Figure 1 presents the comparison between the model predicted bulk settling velocity and the analytical models in equations (2) and (5) above. The hindered settling velocity is determined two ways:

- The slope of the height of the water/solids interface vs time determined during the initial linear settling regime common to batch settling tests.
- The solids velocity measured along the cylinder centreline in the region of uniform settling velocity during the initial linear settling regime.

Figure 1 shows that the centreline velocity tends to better agree with the empirical prediction than the interface velocity. Also, the GTK computational results are in better agreement with the Garside and Al-Dibouni (1997) hindered settling predictions than the original Richardson and Zaki (1954) prediction in eqn (2).

On average the centreline settling velocities are within 5% of the hindered settling velocity relationship using eqn 5. Note, however the settling velocity at 25%v for 1000 micron particles differs by 19% and the predictions at 25% and 50% for 100 micron particles differ by about 10%. The cause of the discrepancy at these points compared to others is not readily understood; further investigation is necessary.

The authors varied the GKT model options and inputs in Table 1, where appropriate, to gauge the impact the selected drag and viscosity models have on the settling velocity results. The settling velocities predicted using the different viscosity and drag models were all within close agreement of the settling velocities in Figure 1. This agrees with Yang (2009) who completed an investigation of the various granular models and parameters available within Fluent (listed in Table 1) and found the settling behaviour of bi-disperse particles to be relatively insensitive to the selected parameters.

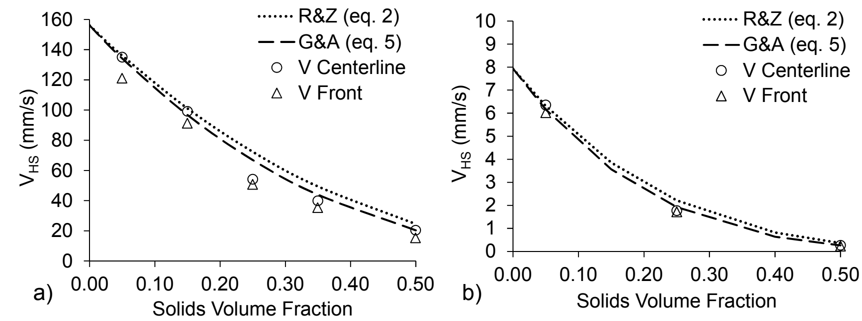

Fig. 1.Comp. of V_{HS} in Newtonian fluid, a) 1000 micron particles, b) 100 micron particles.

2.2 CASE 1B – QUASI-STATIC SETTLING IN VISCOPLASTIC FLUID

Two scenarios arise when considering particle settling behaviour in viscoplastic fluids. When the fluid yield stress is sufficient, the fluid supports the particles and no settling occurs under quiescent conditions. Settling only occurs when the fluid is sheared. When the particle size and density are sufficient, or the yield stress low enough, the particles are able to settle under quiescent conditions.

The criterion detailed in Chhabra (2008) and provided in equation (6) determines whether a particle will settle:

$$Y_G = \frac{\tau_y}{g d_p (\rho_p - \rho_l)}, \qquad (6)$$

where τ_y is the yield stress, g is the gravitational constant, d_p is the particle diameter, and ρ_p and ρ_l are the respective densities of the particle and fluid. The critical value of Y_G has been debated by various researchers and found to vary between 0.048 and 0.212 (Chhabra, 2008). For this discussion, yield stress and particle parameters are chosen to avoid the area of uncertainty within the bounds of the Y_G parameter. The focus of the investigation is on evaluating the GKT model under well behaved conditions.

With a sufficient yield stress, the particle should remain suspended and the settling velocity will be zero. It is immediately clear, without any computational analyses, that in each cell the fluid flow calculations within Fluent utilize an equivalent viscosity. This viscosity is determined based on the current flow conditions and the selected rheological model. This results in a non-zero particle settling velocity regardless of whether the yield stress is sufficient to suspend the particles.

From a purely mathematical viewpoint the numerical implementation is not able to predict the suspension of particles under quiescent fluid conditions. Note however, the resulting apparent viscosity under these suspension conditions is extremely high (10^9 Pa.s typically for even a low yield stress fluid) at low strain rates. This results in settling velocities on the order of 10^{-11} mm/s. Under the time scales of interest in industrial applications, it is appropriate to treat these settling velocities as negligible. So while not strictly mathematically correct, one is able to model particle suspension in viscoplastic fluids using the Fluent rheological implementation.

For a low yield stress below the viscoplastic suspension threshold, the extremely high resulting apparent viscosity ($\sim 10^8$ Pa.s) makes the particle settling negligible for most industrial applications when considering quasi-static flow. The settling behaviour becomes more interesting when the fluid is sheared, and the apparent viscosity is lowered by orders of magnitude, as will be discussed discussed in Section 2.4.

2.3 CASE 2 – SHEAR MIGRATION

The shear particle migration is important in understanding the particle motion within Newtonian and viscoplastic fluids. Several researchers (Bui and Rudman 2003, Ahmad et al., 2010, Tiwari et al., 2009) have successfully modelled the basic shear migration of neutrally buoyant particles using CFD. However, each utilized a direct implementation of user-defined functions to model the effect directly.

Of interest in this study is whether the granular kinetic theory approach is able to predict this behaviour as part of modelling the overall particle motion, without the necessity of incorporating additional diffusive models into the computational scheme.

The GKT implementation within Fluent allows the inclusion of a Saffman lift force component into the granular model. The Saffman lift force on a particle is the lateral lift acting on a particle due to a linear shear flow. In Fluent (2012), the lift force is modelled using equation (7). This evaluation case looks at both the inclusion and exclusion of the Saffman lift force in the GKT model to predict the particle migration under simple shear.

$$\vec{F}_{lift} = -C_L \rho_l \propto_p \left(\vec{v}_l - \vec{v}_p\right) \times (\nabla \times \vec{v}_l) \quad (7)$$

To evaluate the GKT modelling approach, the authors attempted to replicate the experimental shear migration in Newtonian oil reported by Philips et al. (1991). Also of interest is the ability of the model to predict the particle migration in non-Newtonian carrier fluids. For this investigation, the experimental data of Rao et al. (2002) is appropriate. Rao et al. utilized the same test geometry and particles as Philips et al.

Geometry and Material Properties

The wide-gap Couette geometry used by Philips et al. (1991) is modelled for the study. The outer cup diameter is 23.8 mm, the inner cup diameter is 6.4 mm, and the overall sheared length is 250 mm. The inner radius rotates while the outer cup, bottom, and top walls are fixed.While it is possible to model the flow as a 2D axisymmetric model, a full 3D model was utilized in case non uniform particle migration occurred.

Philips tested a suspension of polymethyl methacrylate (PMMA) spheres with density of 1.182 g/cm^3 in a solution of Newtonian oil tailored so the fluid density matched the particle density. The fluid had a viscosity of 4.95 Pa.s. This computational evaluation case aims to replicate Philip's experimental 55% particle volume concentration and 675 mm particle diameter results.

In the experiments, Philips et al. (1991) rotated the inner cylinder over a range of 17 RPM to 117 RPM, resulting in shear rates between 1 and 25 1/s. Philips found that the results were independent of the rotation speed of the inner cylinder. To simplify the comparison matrix, the authors considered only the 117 RPM rotation speed for this evaluation.

Results and Discussion

Figure 2 presents the radial concentration profile predicted from the computational model at 800 spindle revolutions to the data provided by Philips for 50, 100, 200, 800 and 12,000 revolutions. The GTK CFD results, with and without the Saffman force component, are included in the plot. As is clear from the figure, the basic GKT model formulation, with or without the Saffman lift force included, is not able to capture the particle migration due purely to shear.

Rao et al. (2002) utilized an identical experimental set up as Philips et al. (1991), but with a non-Newtonian Carbopol and glycerine mixture as the suspending fluid. The intent of our evaluation was to also compare the computational GKT model results to this test data. However, since the GKT model is not able to replicate the Newtonian flow behaviour, the non-Newtonian case is omitted from the comparison.

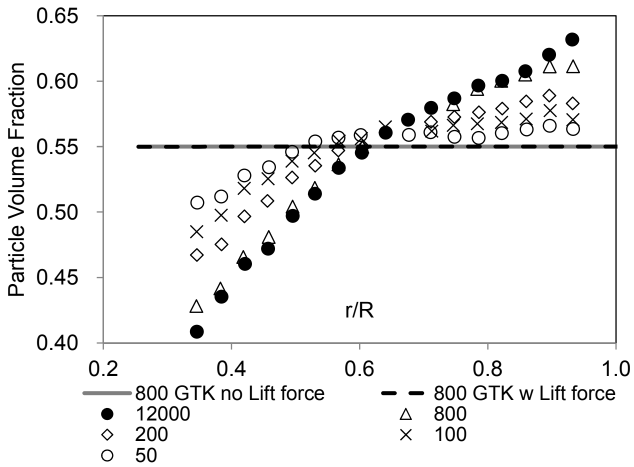

Fig. 2. Comparison of Particle Migration Results

2.4 CASE 3- SHEAR SETTLING

The final evaluation case aims to replicate the experimental non-Newtonian shear settling results of Ovarlez et al. (2012). Similar to Philips et al. (1991) and Rao et al. (2002), Ovarlez also used MRI techniques to determine the velocity and concentration profiles within their Couette flow test apparatus. While Philips et al. (1991) and Rao et al. (2002) were concerned with the radial migration of neutrally buoyant particles, Ovarlez et al. focused on understanding the settling under sheared conditions.

Geometry and Material Properties

Ovarlez et al. (2012) utilized a Couette apparatus with an outer radius of 60 mm, inner radius of 41 mm, and sheared length of 110 mm. The setup also incorporated a 30 mm dead zone at the bottom of the cup where particles could accumulate as they settled. The outer cup was stationary while the inner cylinder rotated at speeds from 5 RPM to 100 RPM. The top fluid surface was open to atmosphere. For this computational investigation the top surface was modelled as a symmetry boundary condition, which provides an acceptable approximation of the free surface for this analysis.

Ovarlez et al. (2012) investigated particle volumetric concentrations ranging from 5% to 40% and four particle diameters. For this evaluation, the authors considered the test results for 275 micron diameter particles at 5% by volume suspended within a concentrated emulsion. The emulsion had a density of 1.0 g/cm^3 and was classified as a Herschel-Bulkley type fluid with τ_y= 8.5 Pa, η_{HB} = 3.6 Pa.s^n, and n = 0.44. The particle's density is 2.5 g/cm^3. The yield suspension criterion in equation (6) indicates that the particles remain in suspension while at rest.

This evaluation considers only the Ovarlez et al.'s (2012) 5% concentration data set for comparison. It is the most complete data set detailed in their study, and the study in Case 1a found the Newtonian quasi-static settling results at 5% agreed well with the empirical solution.

Results and Discussion

As initial validation of the CFD model, the fluid-only radial velocity profiles at various speeds were compared to those reported by Ovarlez et al. (2012) and found to be in close agreement. These comparisons are not shown for brevity.

Figure 3 presents a comparison of the experimental concentration profiles measured by Ovarlez et al. (2012) to those predicted by the GKT computational model.The experimental results show the solids settle in a fairly uniform block with a relatively sharp fluid-solids interface at the top, and only the interface height decreases with time. A sharp increase in solids concentration is observed in the dead zone as solids accumulate.

This behaviour differs from the GKT model prediction, which indicates the formation of a more gradual concentration gradient through the bulk fluid within the sheared zone and the absence of a sharp fluid-solids interface at the top.

Also plotted in Figure 3 are the concentration profiles Ovarlez et al. (2012) predicted from an analytical model they developed to predict the sheared settling behaviour. As with the GKT model, their model also predicts a more gradual concentration gradient through the sheared region than observed in the experimental results. Ovarlez et al. (2012) argue that their analytical model may not account for some of the collective effects of shear rate heterogeneity and the resulting apparent viscosity homogeneity in their theoretical evaluation of the settling.

Ultimately the GKT model predictions mimic the experimental results in rough approximation, but the predictions are far from satisfactory. Further investigation and likely GTK model adaptation are required to better predict the settling behaviour under sheared conditions.

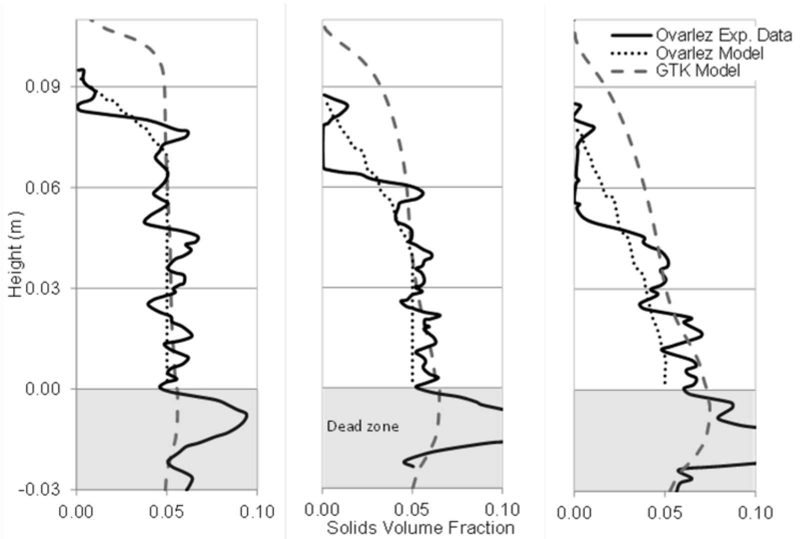

Fig. 3. Comparison of GKT model results to those of Ovarlez et al. (2012) at times of 15 minutes, 30 minutes, and 45 minutes.

3. CONCLUSIONS

The GKT model satisfactorily predicts particle hindered settling in quasi-static Newtonian fluid. The model is fundamentally not able to predict the suspension of particles in viscoplastic fluids of sufficient yield stress. However, in most practical scenarios, the resulting hindered settling velocity is insignificant. The standard GKT model does not appear able to predict the particle migration due to simple shear in Newtonian flows. Consequently no further evaluation is made considering viscoplastic fluids. Of final interest is the ability of the model to predict particle settling in sheared viscoplastic fluids. While the overall settling behaviour is captured, the model predictions differ appreciably from the experimental results. Further investigation and model improvements are therefore required to utilize the GKT Eulerian-Eularian approach for modelling particle motion in viscoplastic fluids.

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