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SMOOTHED PARTICLE HYDRODYNAMICS SIMULATION OF NON-SPHERICAL PARTICLE SUSPENSIONS

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Abstract. Particulate suspensions are used in many technical areas: ceramic processing, powder metallurgy and pharmaceutical applications being only a few examples. In many of these applications the microstructure determines the product quality. To further optimize the production processes a better understanding of the rheological behavior and the microstructure development inside the suspension is needed. Therefore, a direct numerical simulation method taking into account both particle interactions and hydrodynamics has been developed. It is used to investigate the particle orientation during the tape casting of thin ceramic sheets.

1 INTRODUCTION

The rheological behavior and microstructure of a suspension are very important parameters in processes involving suspensions. E.g. in ceramic sheets produced by tape casting [1] an anisotropic micro-texture can be observed: The powder particles in the green tape are aligned in the casting direction [2]. This leads to subsequent undesired anisotropic sintering shrinkage in the later processing of the sheet. The cause for this particle orientation is the shearing of the ceramic slurry below the blade. This has recently been numerically investigated on a macroscopic scale [3].

In order to fully describe and understand such a system, not only a macroscopic but also a microscopic computational fluid dynamics model with fluid-solid coupling as well as the interaction between the particles is needed. As the length scales of the process reach over multiple magnitudes, a multi-scale approach is required. In this paper, the microscopic model and results concerning the motion of non-spherical particles in shear flow will be presented. The macroscopic model can be found in a previous paper [3].

Rigid objects composed of multiple constrained sub-particles have been used in different particle-based, meshfree methods, e.g. the Discrete Element Method (DEM) [4,5] and Dissipative Particle Dynamics (DPD) [6]. As the Smoothed Particle Hydrodynamics (SPH) [7] method is in its main features, e.g. particle-based and meshfree, similar to these it allows an easy implementation of the aforementioned concept for rigid objects. The main features of the model are given in this paper, a more detailed description can be found in [8]. Similar SPH models were published by other groups [9, 10].

2 SIMULATION MODEL

2.1 SPH Implementation

A detailed explanation of SPH used in this paper can be found in Monaghan's review [11]. Therefore, only the basic details of SPH will be described here. SPH is a Lagrangian meshfree method to simulate fluid flows. The fluid is discretized by particles which move with the flow. The particles are not real physical entities but a mathematical form to describe the continuum. Field properties such as density, shear rate, etc. can be calculated through interpolation over the particles. This is done by using a kernel interpolation function with a given range, the so called smoothing length. The equation for the movement of the particles is derived from the Navier-Stokes equation. In this paper the following formulation is used [12]:

$$\frac{d\mathbf{v}_i}{dt} = -\sum_j m_j \left(\frac{p_j}{\rho_j^2} + \frac{p_i}{\rho_i^2} \right) \nabla_i W_{ij} + \sum_j m_j \left(\frac{\mathbf{T}_j}{\rho_j^2} + \frac{\mathbf{T}_i}{\rho_i^2} \right) \cdot \nabla_i W_{ij} + \mathbf{F}_i \tag{1}$$

where v_i is the velocity of particle i (i = 1 … N, N: number of particles), m_i its mass, p_i its hydrostatic pressure, ρ_i its density, T_i the viscous stress tensor at the location of particle i and F_i a body force per unit mass for particle i. W_{ij} is the kernel interpolation function between particles i and j. A cubic spline kernel function and density summation formalism for the continuity equation were used.

2.2 Solid-Fluid Coupling

A rigid body is formed by a constrained cluster of SPH particles. The motion of a rigid body is governed by the summation of all forces on the SPH particles composing the rigid body. In our case these are the standard SPH forces, derived from equation (1). A rigid body motion solver [13] was implemented in our SPH code SimPARTIX.

As there is no contact force other then the SPH forces, overlap in the range of the smoothing length might occur between SPH particles of different rigid bodies. This should influence the results only slightly as the systems we investigate have low particle volume fractions and low Reynolds numbers. In this regime the viscous forces are dominating over the inertia forces.

2.3 Viscosity calculation

The viscosity is calculated through the total stress tensor [14], with an additional term accounting for the constraint forces on the SPH particles composing the rigid body [15].

3 APPLICATION TO SUSPENSION MODELLING

3.1 Jeffery Orbit

The rotation of particles in a shear flow is a first test of the simulation model. Jeffery's equations describe the movement of an ellipsoidal particle in a Stokes flow [16]. This analytical model is used to analyze the results of the simulations. The rotation period with respect to shear rate and particle aspect ratio is given by:

$$T = 2\pi \frac{r_e + \frac{1}{r_e}}{\dot{\gamma}} \tag{2}$$

Here T is the rotation period, r_e is the aspect ratio of the ellipsoids and $\dot{\gamma}$ the shear rate. $r_e = a/b$ where a and b are the axis of the ellipsoidal particle. The simulation setup is chosen in such a way that the simplified 2d form of Jeffery's equations can be used:

$$\phi(t) = \arctan\left(r_e \tan \frac{\dot{\gamma}\, t}{r_e + \frac{1}{r_e}} \right) \tag{3}$$

The setup consists of an ellipsoidal rigid body in a representative volume element (RVE). Through Lees-Edwards boundary conditions (LEBC) a simple shear flow (couette flow) is applied [14]. The orientation of the particle over time is compared to the analytical results of Eq. (3). Different particle shapes and resolutions were simulated. In this paper the results for one shape and three resolutions are shown, an aspect ratio of r_e = 1.44 is chosen as it is close to the particle shapes used in the tape casting process, investigated in [3]. Figure 1 shows the particle with the different resolutions, which, in this case, depends on the smoothing length and also the initial distance between the SPH particles. The initial distance between the particles has been set equal to the smoothing length in the following calculations.

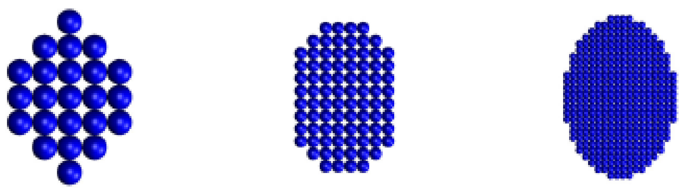

Figure 1: Particle (r_e = 1.44) in three different resolutions (from left to right: smoothing length h: 0.2, 0.1 and 0.05 mm)

The length of the axis a and b of the particle are 1.3 mm and 0.9 mm, respectively. The edge length of the RVE is 5 mm. Viscosity of the surrounding fluid is 3 Pa s. The density was scaled to achieve bigger time steps. All following simulations are in a low Reynolds number regime were the impact of inertia is negligible compared to the viscous forces, thus the scaling of the density will not effect the outcome of the calculations.

In Fig. 2 the results of the simulations are shown as well as the analytical solution of the Jeffery orbit for the aforementioned parameters.

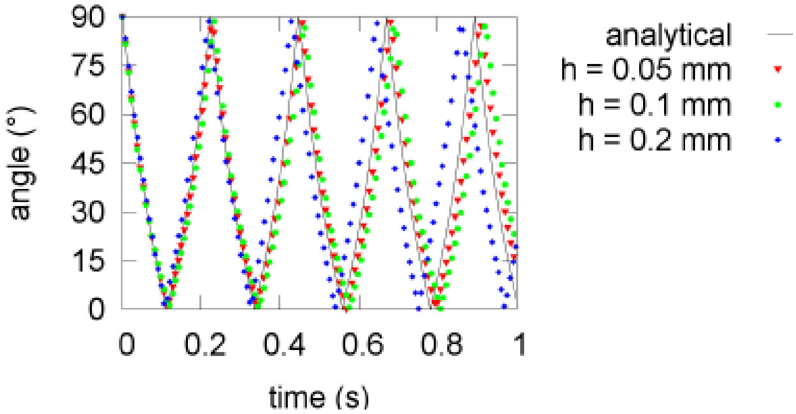

Figure 2: Orientation of the particle depending on the time at $\dot{\gamma}$ = 30 1/s and r_e = 1.44 (an orientation angle of 0° corresponds to a fully horizontally aligned particle)

Not surprisingly the agreement between simulation and the analytical result is best at the highest resolution. At h = 0.1 mm the result is still satisfying, but at h = 0.2 mm the deviation is significant. The qualitative result is in accordance with the Jeffery orbit, but the quantitative result strongly depends on the resolution. However, even at the highest resolution a slight deviation is still visible, in spite of the fact that the shape of the particle is well reproduced. A likely cause for this is the RVE cell, which is small compared to the rigid body. The rotating particle causes perturbations in the flow field, which may lead to locally inhomogeneous shear rates different from the one specified on the LEBC. The shear rate around the particle in Fig. 3 shows the size and magnitude of the perturbation. Also the SPH particles inside the body behave different than normal SPH particles as they are not compressible. Furthermore the accuracy of the boundary between the particles and the fluid depends on the smoothing length (and thus also on the resolution) as SPH particles can overlap to a certain degree. So there is a difference between the volume of a rigid object composed of SPH particles and the effective volume during the simulation. This difference should be proportional to the smoothing length.

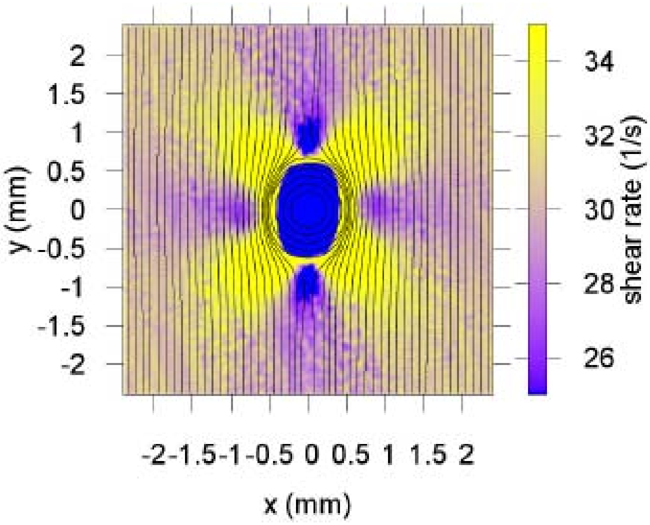

Figure 3: Shear rate and streamlines around the particle

The result of the simulation with 0.05 mm is used to fit the shear rate in Eq. (2) to compensate the effects discussed above. This yields a shear rate of 29.51 1/s and a perfect accordance between the simulation and the analytical result is obtained. As the deviation from the nominal shear rates is small, it is conceivable that the difference is caused by the perturbation of the shear field. This would mean that at this resolution the cell size is the main cause for the deviation between simulation and analytical solution. At lower resolutions the deviation remains important, as it is not only related to the perturbation of the flow field but to the fact that the shape of the particle cannot be resolved accurately at such a coarse resolution.

3.2 Suspension viscosity

The viscosity of a suspension is determined by the viscosity of the solvent and the volume fraction of particles. In the simple case of hard spheres, taking into account the hydrodynamic interactions, the dependency is given by the Batchelor equation [17]:

$$\eta = \eta_s (1 + 2.5\phi + 6.2\phi^2) \tag{3}$$

where η and η_s are the viscosity of the suspension and the solvent, repectivaely. ϕ is the particle volume fraction. This formula is applicable to volume fractions up to $\phi < 0.1$.

Similar to the particle rotation simulations a second RVE was filled to different volume fractions with spherical rigid bodies. Here as before, it has to be taken into account that the effective volume fraction depends on the smoothing length as the SPH particles can overlap during the simulation. A correction term has been applied, taking into account the overlap and the smoothing length when generating the initial simulation setup. Table 1 contains the simulation parameters. Fig. 4 shows the initial state of the simulation with 6 % volume fraction particles.

Table 1: Simulation paramters for the suspension viscosity simulations

Solvent viscosity η_s	4 Pa s
Shear rate $\dot{\gamma}$	5 1/s
Edge length of the RVE d	2.5 mm
Particle size d_p	0.32 mm
Smoothing length h	0.05 mm
Volume fraction ϕ	0, 0.015, 0.03, 0.045, 0.06, 0.075

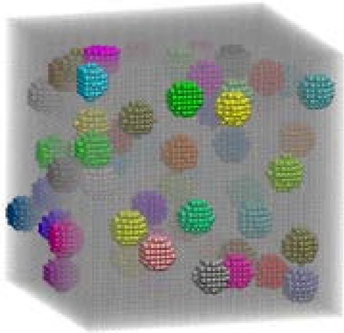

Figure 4: Initial state of the RVE for the simulation with a particle volume fraction of 6 %

The results show a good quantitative agreement with the viscosity predicted by the theory. The comparison can be found in Fig. 5.

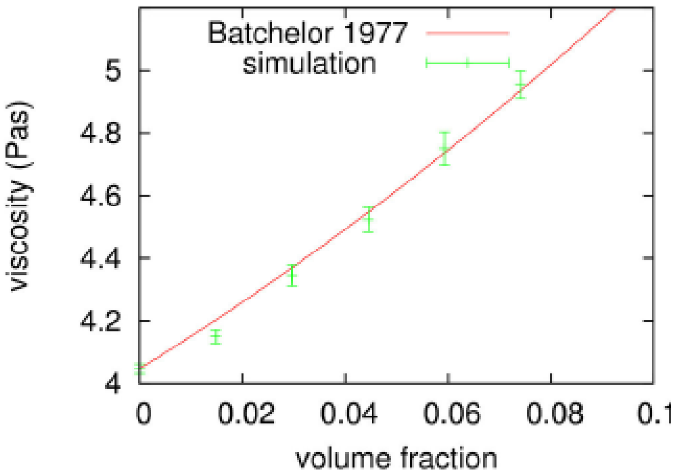

Figure 5: Viscosity in simulation and theory dependent on the particle volume fraction

3.3 Anisotropy development

The rigid body model presented in this work enables the investigation of the movement of the particles inside the slurry on a microscopic scale. The focus is on the orientation of the particles in a shear flow with a volume fraction as typically used for tape casting and different particle aspect ratio. The purpose of these simulations is to investigate the limits of applicability of Jeffery's equation at higher volume fractions. To compare the results the analytical Jeffery's equation was solved numerically for a system with a high number of initially randomly orientated particles with different shapes. Thus, it should be possible to see the effects of the hydrodynamic interactions and particle collision on the orientation of the particles as these are not taken into account in Jeffery's equation.

The simulation setup is identical to those in section 3.2. The main differences are the larger RVE to particle size ratio and the use of non-spherical particles. Three particle aspect ratios were used. All parameters were chosen in the range typically used in tape casting. The parameters can be found in Table 2.

Table 2: Simulation parameters for the orientation simulations

Solvent viscosity η_s	0.42 Pa s
Shear rate $\dot{\gamma}$	60 1/s
Particle size d	35 µm
Smoothing length h	4 µm
Volume fraction ϕ	22 %
Aspect ratio r_e	1.0, 1.25, 1.5

Fig. 6 shows the results of the simulations. Periodic oscillations are visible on the solid line showing the momentary average orientation. As the systems consist of about 180 particles the curve is not smooth as the amount of particles is not sufficient to get satisfying statistics. The dashed line is the running average, which can be used to compare the results of the simulation with the analytical calculation. In Table 3 the results for both are shown. As the differences between the analytical calculation and simulation are small, it is reasonable to assume that the particles are not significantly disturbed by interaction with other particles in their rotation, at least for the volume fraction and particle shapes studied here. At higher aspect ratio the difference becomes higher, one explanation for this behaviour is that the more elongated the particles are the higher the chance that they hinder each other in their rotation. This might not be applicable to particles with even higher aspect ratios then those studied in this work, as other effects might influence the particle orientation in these areas. To make a more general statement concerning the behaviour of particulate suspensions, the system has to be investigated in more detail over a broader range of particle shapes and volume fractions.

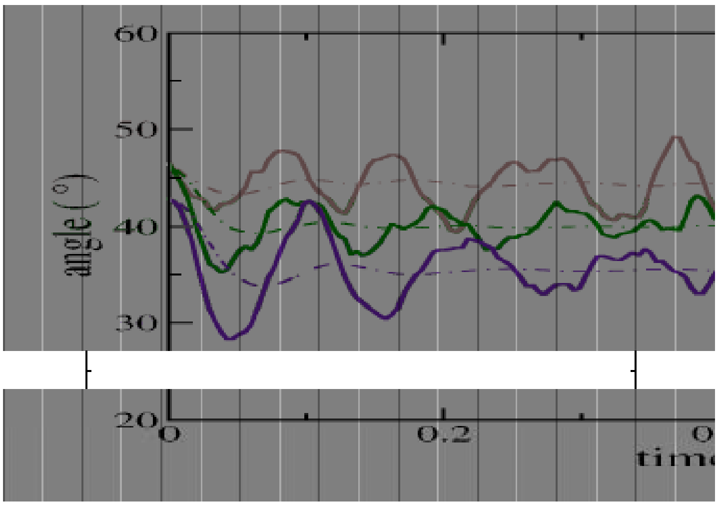

Figure 6: Average (solid line) and running average (dashed line) orientation of the particles depending on the aspect ratio (an orientation angle of 45° corresponds to a system with a random particle orientation, lower angles to a horizontal alignment and higher angles to vertical alignment)

Table 3: Comparison between numerically and analytically calculated average particle orientation

r_e	ϕ_{theory}	ϕ_{sim}
1.0	45.00°	45.69°
1.25	49.10°	50.08°
1.5	52.24°	54.41°

4 SUMMARY AND OUTLOOK

An SPH simulation model with solid-fluid coupling for suspensions with non-spherical particles has been developed. Different verification tests have been made, which show a good agreement with theoretical predictions. The model was then used to investigate the influence of the particle shape on the orientation of particles in flow conditions which are typical for tape casting. It has been shown that the orientation in the green tape is linked to the rotation of the particles in the shear field under the blade. The orientation of the particles depends on the particle shape and the volume fraction. The analytical Jeffery's equation for the rotation of the particles seems to give a good estimate for the particle alignment at least for volume fractions below 25% and small particle aspect ratios. At the highest particle ratio used in this work the Jeffery's equation underestimates the orientation.

In future, the model will be enhanced to be able to simulate more complex suspensions. In realistic suspension the short range van der Waals forces, which draw the particles together, are counteracted by electrostatic or steric forces which stabilize the suspension. Also more precise contact forces, as those typically used in DEM simulation, will be implemented to describe the collisions between rigid bodies more thoroughly. This should also enable an even more detailed modeling of the slurries used in tape casting.

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REFERENCES

[1] Mistler, R.E., Twiname, E.R. *Tape casting: Theory and Practice.* American Ceramic Society, Westerville, OH (2000)

[2] Besendörfer, G., Roosen, A. Particle shape and size effects on anisotropic shrinkage in tape-cast ceramic layers. *J. Am. Ceram. Soc* (2008) **91**(8):2515-2520

[3] Wonisch, A., Polfer, P., Kraft, T., Dellert, A., Heunisch, A. and Roosen, A. A comprehensive simulation scheme for tape casting: From flow behavior to anisotropy development. *J. Am. Ceram. Soc* (2011) in press

[4] Favier, J.F., Abbaspour-Fard, M.H., Kremmer, M. et al. Shape representation of axisymmetrical, non-spherical particles in discrete element simulation using multi-element model particles. *Eng. Computation* (1999) **16**(4) :467-480

[5] Bierwisch, C., Kraft, T., Riedel, H., Moseler, M. Three-dimensional discrete element models for granular statics and dynamics of powders in cavity filling. *J. Mech. Phys. Solids* (2009) **57**(1):10-31

[6] Hoogerbrugge, P.J., Koelman, J.M.V.A. Simulating microscopic hydrodynamic phenomena with dissipative particle dynamics. *Europhys. Lett* (1992) **19**(3):155-160

[7] Gingold, R.A., Monaghan, J.J. Smoothed particle hydrodynamics – Theory and application to non-spherical stars. *Month. Not. R. Astron. Soc.* (1977) **181**(2):375-389

[8] Polfer, P. *Entwicklung und Anwendung eines mehrskaligen Simulationsmodells für das Foliengießen von Keramikschichten.* diploma thesis, Karlsruhe Institut für Technologie (KIT), Germany, (2009)

[9] Potapov, A.V., Hunt, M.L. and Campbel, C.S. Liquid-solid flows using smoothed particle hydrodynamics and the discrete element method. Powder Technol (2001) **116**:204-213

[10] Martys, N.S., George, W.L., Chun, B., Lootens, D. A smoothed particle hydrodynamics-based fluid model with a spatial dependent viscosity: application to flow of a suspension with a non-Newtonian fluid matrix. *Rheol. Acta* (2010) **49**:1059-1069

[11] Monaghan, J.J. Smoothed particle hydrodynamics. *Rep. Prog. Phys* (2005) **68**:1703-1759

[12] Sigalotti, L.D., Klapp, J., Sira, E., Melean, Y. and Hasmy, A. SPH simulation of time-dependent poiseuille flow at low Reynolds numbers. *J. Comp. Phys* (2003) **191**(2):622-638

[13] Omelyan, I.P. On the numerical integration of motion for rigid polyatomics: The modified quaternion approach. *Comput. Phys* (1998) **12**(1):97-103

[14] Allen, M.P., Tildesley, D.J. *Computer simulations of liquids*. Oxford University Press, U.S.A., (1997).

[15] Martys, N.S., Mountain, R.S. Study of dissipative-particle-dynamic-based model of suspensions. *Phys. Rev. E* (1999) **59**:3

[16] Jeffery, G.B. The motion of ellipsoidal particles immersed in a viscous fluid. *Proc. R. Soc. Lond. A* (1922) **102**(715):161-179

[17] Batchelor, G.K. The effect of Brownian motion on the bulk stress in a suspension of spherical particles. *J. Fluid. Mech* (1976) **83**:97-117