

DISCRETE ELEMENT MODELLING OF NON-SPHERICAL PARTICLES IN TURBULENT GAS-SOLID FLOWS

Berend van Wachem¹, Victor Chéron², Fabien Evrard^{2,3}

¹Corresponding Author. E-Mail: berend.vanwachem@ovgu.de. Chair of Mechanical Process Engineering, Faculty of Process and Systems Engineering, Otto-von-Guericke University Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany
² Chair of Mechanical Process Engineering, Faculty of Process and Systems Engineering, Otto-von-Guericke University Magdeburg,

Universitätsplatz 2, 39106 Magdeburg, Germany

³ Sibley School of Mechanical and Aerospace Engineering, Cornell University, Ithaca, NY 14853, United States of America.

ABSTRACT

In this contribution, a CFD/DEM framework is introduced to predict the behaviour of non-spherical particles in (turbulent) flows. This computational framework comprises different elements. Firstly, the drag, torque and lift relations of each particle shape is determined by means of true direct numerical sim*ulation*, where the particle is represented by a highly accurate immersed boundary method. Secondly, to deal with particle-particle and particle-wall interactions, a collision model is derived to deal with the collisions between non-spherical particles and the particles and a wall. The discrete element framework is constructed based upon a Quaternion approach. Finally, the framework is tested on two different testcases: the first is a horizontal channel flow with fibers and the second one is a fluidized bed with ellipsoidal particles. In general, the results show that there is a big effect of particle shape and particle-orientation, which can be accurately captured by the presented framework.

Keywords: CFD/DEM, Direct numerical simulation, Discrete element method, Immersed boundary method, Non-spherical particles

NOMENCLATURE

Ī	$[kg m^2]$	moment of inertia
F_D	[N]	particle drag force
F_L	[N]	particle lift force
\boldsymbol{F}_n	[N]	normal collision force
\boldsymbol{F}_t	[N]	tangential collision force
Κ	[]	spring constants
V_p	$[m^3]$	particle volume
a_c	$[m/s^2]$	particle acceleration due to
		collisions
a_p	$[m/s^2]$	net particle acceleration
g	$[m/s^2]$	gravity acceleration
е	[-]	coefficient of restitution
q	[-]	quaternion

t	[<i>s</i>]	time
δ	[m]	displacement
ω	[rad/s]	particle rotation
ρ_p	$[kg/m^3]$	particle density
τ	[N m]	torque

Subscripts and Superscripts

b body space

1. INTRODUCTION

The knowledge of the dynamics of turbulent gassolid flows has an even increasing importance for the successful design, improvement and operation of numerous industrial applications in process industry, such as fixed and fluidized bed reactors, pneumatic conveying, cyclones, biomass combustors, to just name a few. Such systems exhibit very complex flow dynamics and interactions between the particles and the gas-phase turbulence, also including particleparticle and particle-wall interactions.

The majority of studies involving gas-particle flows assume that particles are perfect spheres. This assumption is very convenient because of several factors: perfect spheres are simple to model, their behavior is well known, and there is a large availability of models in the literature which describe the particle-fluid interactions e.g.[1]. However, assuming the particles are perfect spheres may be unrealistic, because most applications deal with nonspherical particles. Analysis of flows with nonspherical particles is considerably more complicated than flows with spherical particles. While a sphere is characterized by its diameter only, even a very simple non-spherical particle such as a disc or a fiber needs at least two parameters to be uniquely defined. This makes the rigid body dynamics of non-spherical particles more complex than that of spherical ones. Moreover, additional complexities arise in describing the interaction of a non-spherical particle with a fluid.

In a uniform flow, the dominant force on a sphere is the drag force, whereas a non-spherical body can also be affected by a transverse lift force, a pitching torque and a counter-rotational torque [2]. Moreover, all of these forces acting on a non-spherical body depend not only on the Reynolds number, but also on the angle between the axes of the particle and the direction of the incoming flow. Additionally, the framework for describing collisions requires a different approach compared to the one used for perfect spheres; for instance, it needs to take into account the orientation of the particle.

The aim of this contribution is to present a framework, based on computational fluid dynamics (CFD) and the discrete element method (DEM), to be able to predict the behavior of non-spherical particles in (turbulent) fluid flows. This framework consists of multiple numerical aspects: first, we will use a novel immersed boundary method (IBM) framework to determine the hydrodynamic behavior of a single non-spherical particle under varying conditions. Secondly, we will propose a DEM framework to model the behavior of non-spherical particles based upon the concept of Quaternions. Finally, we will bring together the resulting drag, lift and torque model obtained from the IBM simulations and the DEM framework into a single CFD/DEM framework to predict the behavior of non-spherical particles. To show the ability of the complete framework, two test-cases are presented: the first is the flow of nonspherical particles in turbulent channel flow, and the second is a small fluidized bed with non-spherical particles.

2. IMMERSED BOUNDARY METHOD

The immersed boundary method (IBM) is a popular and efficient way to mimic the behaviour of a boundary condition on a fixed Eulerian mesh. There are a number of implementations of the IBM, falling into, broadly speaking, three categories: cut-cell IBM [3], the ghost-cell IBM [4], and the direct forcing IBM [5]. In this contribution, we adopt the direct forcing IBM as described in [5], which uses an efficient and strong flow-particle coupling scheme. This implementation includes a stabilisation strategy, which scales the forcing weights automatically, in order to create an optimal forcing, minimizing the transpiration error whilst remaining stable.

For each particle shape, many simulations are carried out, where the particle Reynolds number is varied between 0.1 and 500, and the angle of attack is varied. Examples of such simulations are shown in Figure 1 for an ellipsoid and Figure 2 for a fiber. For each simulation, the forces and torques are computed. These forces and torques are then used to design shape-specific correlations, that describe the interactions between the fluid and the particles. The equations are used as a base of large-scale analysis of complex flows with non-spherical particles.



Figure 1. A snapshot of the resolved flow around an ellipse.



Figure 2. A snapshot of the instantaneous velocity (stream plots) and pressure field (color) in a flow past a fiber of aspect ratio 5 at particle Reynolds number 300 and angle of attack $\phi = 30$.

3. DEM: DYNAMICS OF NON-SPHERICAL PARTICLES

Although the motion or dynamics of a spherical particle is relatively straightforward [6], the dynamics of a non-spherical particle are more complicated. The rigid body dynamics of a non-spherical particle concern its motion and behaviour during one or more collisions. The ordinary differential equation describing the translational position and velocity are the same as for a spherical particle (Newton's second law), as given in the framework of DEM [7]:

$$\frac{D\boldsymbol{v}_p}{Dt} = \boldsymbol{a}_p \tag{1}$$

$$\rho_p V_p \boldsymbol{a}_p = \underbrace{\boldsymbol{F}_D}_{\text{drag}} + \underbrace{\boldsymbol{F}_L}_{\text{lift}} + \underbrace{V_p \rho_p \boldsymbol{g}}_{\text{gravity}} + \underbrace{V_p \nabla P}_{\text{Archimedes}} + \underbrace{\rho_p V_p \boldsymbol{a}_c}_{\text{collisions}}$$
(2)

where V_p is the volume of the particle, ρ_p the density, v_p the velocity of the particle in the *Lagrangian* framework, and a_c represents the acceleration of the force arising from collisions between particles. The added mass and history forces are neglected in the equation, as they are not significant in the case studied in this contribution.

The rotational motion of a non-spherical particle is very different compared to that of a spherical particle. For a non-spherical particle the orientation is important, unlike for a spherical particle. To derive the rotational equations of motion for a non-spherical particle, it is convenient to introduce two types of Cartesian space: body space and world space. Calculations are performed in either space. These two Cartesian spaces are shown in Figure 3.



Figure 3. The relation between body space (a) and world space (b). The fixed axes of body space, x^b , y^b and z^b are indicated in both figures. The position of a fixed point in body space, p^b is transformed to world space, p(t).

Due to the absence of singularity and Gimbal lock problems [8], unit Quaternions are increasingly popular to represent the rotation of a non-spherical particle. General Quaternions do not only change the orientation of a vector, but also scale the length of a vector. Therefore, the equation for representing rotation cannot be a simple Quaternion multiplication, as the length of the vector could change. To represent rotation by Quaternions, the length of the Quaternions must be exactly unity. Rotation without scaling is performed by unit Quaternions [9].

3.1. Quaternions

A quaternion consists of 4 numbers and represents the rotation and scaling of a body [10]. A quaternion with unit length represents an arbitrary rotation without scaling in 3D space. The condition of the unit length reduces the number of degrees of freedom from 4 to 3. The ODE of a quaternion is similar to that of a rotation matrix,

$$\dot{q}(t) = \frac{1}{2}\omega(t)q(t) \tag{3}$$

The rotation of a body can be seen as the subsequent application of two rotations, given by a pair of quaternions. Thus, the quaternion at the new time level can be interpreted as the quaternion of the previous time level multiplied by the rotational displacement during the time step. The infinitesimal displacement during the time step, is evaluated at the intermediate time level to comply with the mid-point rule and is determined as

$$q_{n+\frac{1}{2}}' = \left[\cos\frac{\|\omega_{n+\frac{1}{4}}\|\delta t}{4}, \sin\frac{\|\omega_{n+\frac{1}{4}}\|\delta t}{4}\frac{\omega_{n+\frac{1}{4}}}{\|\omega_{n+\frac{1}{4}}\|}\right]q_n$$
(4)

Hence, it is necessary to determine the mid-point angular velocity between two adjacent time steps. To get an estimate of the angular velocity for a general non-spherical particle, the equation for angular acceleration can be approximated in body space by

$$\dot{\omega}^{b} = \overline{\overline{I^{b}}}^{-1} (\tau^{b} - \omega^{b} \times \overline{\overline{I^{b}}} \omega^{b})$$
(5)

The moment of inertia in body space is constant, and is expressed as \overline{I}_o , and the relation between the moment of inertia in body space and world space can be represented in quaternion space as

$$\overline{\overline{I}}^{-1} = \left[q(t) \left(q(t) \overline{\overline{I}}_0 q(t)^{-1} \right)^T q(t)^{-1} \right]^T$$
(6)

3.2. Collision detection

At sufficient high particle loading, both particleparticle and particle-wall collisions are important for predicting the behaviour of the flow. Therefore, all potential collisions must be correctly detected in order to determine their contribution. Moreover, the particle-wall collisions are required to keep the particles in the domain. There are various frameworks to describe particle collisions. In the hardsphere, or event driven, framework the collisions are dealt with using global conservation of momentum and energy [6]. In the soft-sphere framework, the dynamics of the actual collision are resolved, using approximations from elasticity theory [7].

In this contribution, we consider the soft-sphere approach, thus contact forces and torques are determined for particles which are actually slightly overlapping. This overlap is a representation for the local deformation, or displacement, and a Hertzian force model can be used to predict the resulting repellent force. Therefore, each pair of near-neighbour particles is checked for overlap. In this contribution, we have chosen to represent each particle as a collection of spheres [11]. This is achieved by 'filling' each body with a number of overlapping fictitious spheres, typically with varying radii, where the number of fictitious spheres determines the accuracy of the surface representation of the body. An example is shown in Figure 4. This framework allows for a similar contact detection approach as for spherical particles, as described, for instance, in [12].



Figure 4. An example of the body shown in Figure 3 filled with 8 spheres. The spheres are used to find potential contact points with neighbouring particles or walls.

3.3. Collision forces

Once a collision is detected, the overlap, or the displacement, between two particles or a particle and a wall is determined. This overlap is used as a meas-

ure to estimate the local deformation of the particle at the point of collision, by assuming the contact point is locally axi-symmetric with a constant local radius, and leads to normal and tangential forces based upon [13],

$$F_n(t) = K_n(t)\delta_n^{\frac{1}{2}}(t)\boldsymbol{n}(t)$$

$$F_t(t) = \min\left(\mu F_n(t), K_t(t)\boldsymbol{\delta}_t(t)\right)$$

where μ is the coefficient of friction, $\delta_n(t)$ is the scalar representing the normal displacement, $\delta_t(t)$ is the vector representing the accumulated tangential displacement over the duration of the collision, mapped onto the current reference frame. The tangential displacement vector is determined by integrating the successive tangential displacements and mapping this into the current frame of reference of the collision. K_n and K_t are the spring constants for the normal and tangential forces respectively, as predicted Hertzian contact theory [13]

$$K_{n,l}(t) = \frac{4}{3}E^* \sqrt{r(t)}$$
$$K_t(t) = 8G^* \sqrt{r(t)\delta_t(t)}$$

where E^* represents the Young's modulus of the pair of colliding particles, G^* is the ratio of the Young's modulus and Poisson's ratio plus one for the pair of colliding particles, r(t) represents the local radius of the particle (the distance from the centre of mass of the particle to the contact point) and the subscript lrepresents the loading, *i.e.* the particles moving towards each other. When the particles move away from each other, the subscript u, representing unloading are used. To account for the dissipative nature of the collision, a coefficient of restitution is introduced to determine the spring constant value for unloading, represented by the subscript u, following [14]

$$e = \sqrt{\frac{K_{n,u}}{K_{n,l}}} \tag{7}$$

The total force on the body is determined by adding the gravity force, the fluid force, and summing the force contributions of all collisions of each particle

$$\boldsymbol{a}_{p}(t) = \boldsymbol{g} + \frac{\boldsymbol{F}_{f}(t)}{m_{p}} + \sum_{c=\text{contacts}} \frac{\boldsymbol{F}_{n,c}(t) + \boldsymbol{F}_{t,c}(t)}{m_{p}} \quad (8)$$

where m_p indicates the mass of the particle, g represents the gravitational acceleration, F_f represents the total interaction force with the fluid, and $F_{n,c}$ and $F_{t,c}$ represent the normal and tangential forces from the collision of the particle.

The torque on the body is determined by adding the torque arising from the fluid and the contributions of all collisions of each particle

$$\boldsymbol{\tau}(t) = \boldsymbol{\tau}_{f}(t) + \sum_{c=\text{contacts}} \left(\boldsymbol{p}_{c} - \boldsymbol{x}_{p}(t) \right) \times \left(\boldsymbol{F}_{n,c}(t) + \boldsymbol{F}_{t,c}(t) \right)$$
(9)

where p_c is the point of contact of the particle with another particle, and x_p is the centre of mass of the particle.

3.4. Hydrodynamic forces and torques

The fluid exerts two types of forces on the particle: drag force in the direction of the flow velocity and a transverse lift force. Additionally, a pitching and counter-rotational torques are present. These interactions are given by the following equations [2]:

$$F_D = C_D \frac{1}{2} \rho \tilde{\nu}^2 \frac{\pi}{4} d_p^2 \tag{10}$$

$$F_L = C_L \frac{1}{2} \rho \tilde{v}^2 \frac{\pi}{4} d_p^2 \tag{11}$$

$$\tau_P = C_T \frac{1}{2} \rho \tilde{\nu}^2 \frac{\pi}{8} d_p^3 \tag{12}$$

$$\tau_R = C_R \frac{1}{2} \rho \left(\frac{d_p}{2}\right)^3 |\mathbf{\Omega}| \mathbf{\Omega}$$
(13)

where F_D are the drag force, F_L is the lift force, τ_P is the pitching torque, τ_R is the rotational torque, C_D , C_L , C_T and C_R are the shape specific force and torque coefficients, $\tilde{v} = \tilde{v}^f - v_p$ is the velocity of the particle relative to the local undisturbed fluid velocity, ρ is the fluid density, and d_p the equivalent particle diameter, *i.e.* the diameter of a sphere with the same volume as the considered particle. The relative rotation of the particle with respect to the fluid is given by

$$\mathbf{\Omega} = \frac{1}{2} \nabla \times \tilde{\mathbf{v}} - \boldsymbol{\omega}_p \tag{14}$$

with ω_p representing the angular velocity of the particle. The total fluid induced force is determined by adding the drag and lift forces and the total fluid induced torque is determined by adding the two torques.

4. CFD: FLUID PHASE MODELLING

The simulations are carried out with our in-house multiphase CFD code Multiflow, which is a transient, three-dimensional, fully coupled parallel computational fluid dynamics (CFD) code based on finite volume discretisation [15, 16] and various types of particle and fluid models. It has shown to be a robust solving framework for viscous multiphase flows in the presence of large source terms and large gradients in density and volume-fraction.

4.1. Large eddy simulation (LES) modelling

The filtering procedure for LES can be found in [17]. The equations arising from filtering are very similar to the Navier-Stokes equations, except for the addition of one term, which describes the behaviour of the sub-grid scale stresses, namely τ_{ii}^a

$$\tau_{ij}^a = \rho_f(\widetilde{v_{f,i}}\widetilde{v_{f,j}} - \widetilde{v}_{f,i}\widetilde{v}_{f,j}) \tag{15}$$

To close the sub-grid-scale stresses, the Smagorinsky model [18] is used. The Smagorinsky model assumes that the local SGS stresses are proportional to the local rate of strain of the resolved flow [19]. The stresses are given as

$$\tau^a_{ij} = -2\mu_{SGS}\widetilde{S}_{ij} + \frac{1}{3}\tau_{ll}\delta_{ij} \tag{16}$$

where $\widetilde{S}_{ij} = \frac{1}{2} \left[\frac{\partial \widetilde{v}_{f,i}}{\partial x_j} + \frac{\partial \widetilde{v}_{f,j}}{\partial x_i} \right]$. and μ_{SGS} is the sub-grid scale eddy viscosity. By analogy to Prandtl's mixing-length hypothesis [20], μ_{SGS} can be estimated as

$$\mu_{SGS} = \rho_f (C_{SGS} \Delta)^2 \sqrt{2\widetilde{S}_{ij} \widetilde{S}_{ij}}$$
(17)

where C_{SGS} is the Smagorinsky constant and Δ is the LES filter width.

It is well-known that the Smagorisnky model is not suitable for accounting for the effect of walls. This is because the no-slip boundary condition at the wall causes a strong velocity gradient (i.e. the Reynolds number near the wall decreases since the velocity drops). From Prandtl's mixing-length hypothesis this would create unrealistic non-zero sub-grid viscosity values and hence shear stresses near the wall [20]. Therefore, a damping function is used to turn-off the μ_{SGS} near the wall; C_{SGS} is modified as

$$C_{vD} = C_{SGS} \Delta (1 - e^{-y^+/A_o^+})$$
(18)

Note that $y^+ = \frac{u_{\tau}y}{v_f}$; where y^+ is the dimensionless distance to the wall, u_{τ} is the friction velocity and A_o^+ is a constant normally taken to be 25. μ_{SGS} is modified as

$$\mu_{SGS} = \rho_f C_{\nu D}^2 \sqrt{2\widetilde{S}_{ij}\widetilde{S}_{ij}}$$
(19)

The model has proved to be quite successful in many types of wall bounded turbulent flows with steady boundary layers [21]. However, a DNS resolution is required in the wall region.

5. CFD/DEM: COUPLING BETWEEN CFD AND DEM

As the particles move in a Lagrangian framework and the fluid is solved in a fixed Eulerian framework, the coupling between these frameworks requires special attention. The fluid velocity as determined on the Eulerian mesh must be accurately interpolated to each of the Lagrangian particles. Some properties of interpolation schemes between the Eulerian and the Lagrangian frameworks are discussed in [22]. A frequently used interpolation scheme is the tri-linear interpolation, which has a number of favourable properties, such as continuity and ease of implementation, but suffers from a strong filtering of higher frequency velocity fluctuations and is probably not suitable for accurate computations. Therefore, we have used a polynomial spline interpolation, where a property of the fluid at the particle is approximated by

$$\phi_{f@p} = \sum_{n=1}^{N} \sum_{i,j,k}^{I,J,K} a_{n,ijk} \Delta x^i \Delta y^j \Delta z^k \phi_{f,n}$$
(20)

where the summation over *n* is over the independent points and the summation over (i, j, k) is over the polynomial integer values, and $a_{n,ijk}$ is the constant coefficient corresponding to independent point *n* and the polynomial powers of (i, j, k) for the three independent directions. The number of independent fluid velocity points, *N*, used to evaluate the spline is 27, and the order of the polynomial used is, therefore (I, J, K) = (3, 3, 3).

6. SIMULATIONS

6.1. Test-case 1: Turbulent channel flow

In this work, the properties of the fluid phase and the computational domain are the same as in the work of Marchioli et al. [23], who have studied this channel case for spherical and ellipsoidal particles. The size of the channel computational domain is $4\pi h \times 2\pi h \times h$ in the x, y, and z directions, respectively, in which h = 0.02 m is the half height of the channel, and the mean flow is in the x direction. There are solid walls in the low and high y directions, and in all other directions, periodic boundaries are applied. Within the turbulent channel flow, fibers with a Stokes number of 5 are released.

In this abstract we show the fluid velocity in the stream-wise velocity in a plane close to one of the walls in Figure 5. Full results are presented during the presentation.



Figure 5. The instantaneous fluid velocity (indicated by colour) in the stream-wise direction and the distribution of ellipsoids with St = 5 and an aspect ratio of 5 near the cross-sectional *x*-*z* plane at $y^+ = 8$.

6.2. Test-case 2: Fluidized Beds

The fluidized bed test-case is from [6] and consists of a quasi-two dimensional fluidized bed of 500 mm high, 90 mm wide, and 8 mm deep filled with ellipsoidal particles of around $d_p \approx 1.75$ mm. The experiments as well as the simulations with spherical particles has been described in [6]. Figure 6 shows a shapshot of the ellipsoidal particles being fluidized in the bed. Full results are presented during the presentation.



Figure 6. An instantaneous snapshot of the position of the ellipsoids in the fluidized bed. The ellipsoids are coloured by their velocity.

7. CONCLUSIONS

In this contribution we present a fully coupled CFD/DEM framework to predict the behaviour of non-spherical particles in flows. We first use a stateof-the-art immersed boundary method to determine the drag, torque and lift of the non-spherical particle shape. We then use a discrete element model to predict the collisions between two particles and particles and a wall. The orientation of the particle in the discrete element model is described in the framework of Quaternions. Finally, two different applications of the coupled CFD/DEM framework are presented: the flow of fibers in turbulent channel flow, and the behaviour of ellipsoidal particles in a fluidized bed. In both simulations, there is a clear preferred orientation of the particles, leading to a significantly different behaviour of the system compared to the system with spherical particles.

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