Modeling the agglomeration of electrostatically charged particles

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Abstract. The agglomeration of particles during the handling of powders results in caking, lumping or the local accumulation of electrostatic energy. In the case of dry powders the attraction in-between particles can be mainly attributed to van der Waals and electrostatic forces. In this paper we present a novel numerical approach which is based on an algorithm developed by Erleben [1] in the field of computer graphics. This algorithm is extended to compute binary and multiple particle interaction with each other and solid surfaces. The herein presented results demonstrate that this algorithm allows to accurately and efficiently predict whether particles agglomerate or separate depending on their kinetic parameters. Simulated test cases reveal how electrostatic and van der Waals forces lead to the growth of structures in case the particle restitution coefficient is sufficiently low.

1. Introduction
A wide range of literature has been contributed to the settling of particles on surfaces. For example reviews Guha [2] the experimental and numerical efforts regarding the physical mechanisms responsible for the deposition of particles. However, this review focuses on airborne particles and does not tackle the actual deposition process, i.e. the forces acting during the contact of a particle with another object. In a similar fashion, Narayanan et al. [3] identified different deposition patterns on the surface of a channel depending on the particle relaxation time. Also the authors of the present paper and co-workers conducted an amount of numerical investigations with focus on the behavior of charged particles [4–6]. In all of these studies the assumption of binary particle interaction was taken which prevents the establishment of a connected agglomeration of several particles.

The development of wall layers due to triboelectric charges in a fluidized bed was recently observed by Sippola et al. [7] through a combined experimental and numerical study. Their simulation included electrostatic and contact forces and enabled the prediction of the amount of stable layers. However, their model did not predict a completely static structure at the wall which resulted in a small residual velocity of particles belonging to an immobile deposit. Recently, Ray et al. [8] implemented a more detailed concept of wall layer formation in an Eulerian-Eulerian framework. They determined if a particle placed in a certain distance from the wall would have enough electrostatic force acting on it such that friction could resist dropping due to gravity. Song and Mehrani [9] proposed a phenomenological model of wall layer development on a gas-solid fluidization column due to electrostatic charges based on their experimental investigations. The model indicated that particle migration towards the wall was due to image and electrostatic forces. However, if a deposit or an agglomeration forms the details of the underlying process become very complicated. One complication arises from the fact that particles in contact pose contact forces on each other which lead to statically over-determined systems.

To sum up, to the best of our knowledge no comprehensive theoretical model of the particle deposition process was formulated yet. However, in the field of computer graphics an efficient algorithm appeared [1] which enables the efficient and accurate tracking of the dynamics of a large number of bodies. In this paper we extend the algorithm of Erleben [1] to compute binary and multiple particle interaction accounting besides for van der Waals and electrostatic forces also for collisional forces and plastic particle deformation.
2. Numerical computation of the dynamics of particle agglomerations

The trajectory of each individual particle is described by Newton’s second law of motion,

$$\frac{d\mathbf{u}_p}{dt} = \mathbf{f}_{ad} + \mathbf{f}_g + \mathbf{f}_{el} + \mathbf{f}_{vdW} + \mathbf{f}_c. \quad (1)$$

In this equation $\mathbf{f}_{ad}$ is the acceleration of the particle by the attacking aerodynamic force, $\mathbf{f}_g$ by gravitation, $\mathbf{f}_{el}$ by electric field forces, $\mathbf{f}_{vdW}$ by van der Waals forces, and $\mathbf{f}_c$ is the acceleration during contact e.g. with other particles or a surface. The force acting on a particle by the electric field is given by

$$\mathbf{f}_{el} = \frac{Q\mathbf{E}}{m_p}, \quad (2)$$

where $\mathbf{E}$ is the local electric field strength and $m_p$ and $Q$ is the mass and the charge of the particle, respectively. Since we focus in the current study on the adhesion process and the formation of deposit layers on surfaces, van der Walls forces between two spherical particles $(i$ and $j)$ in close proximity are computed adopting the model of Hamaker $[10]$,

$$F_{vdW} = -A_H \frac{32}{3} \frac{R_i^3 R_j^3 (R_i + R_j + a)}{(2R_i + a)^2 (2R_j + a)^2 (2R_i + a)^2 a^2}, \quad (3)$$

where the distance between the surfaces of the particles, $a$, is limited by $a \geq 1 \text{Å} = 10^{-10} \text{m}$ and $A_H$ is the Hamaker-Constant which we chose in the present study to be $6.5 \times 10^{-20}$ J.

However, also the sticking of particles to other objects poses contact forces which act as constraints to the future particle dynamics. Since the number of possible contact points within one cluster scales with $(N^2 + N)/2$ (where $N$ is the number of contained particles) the problem of solving the particle trajectories becomes fast numerically impossible when the cluster grows. Therefore, we adopt the method of Erleben $[11]$ which allows to track all particles in Cartesian coordinates. Their motion in a Lagrangian system is given by the equation

$$\mathbf{M} \frac{\partial}{\partial t} \ddot{\mathbf{u}} = \mathbf{J}^T \lambda \dot{\lambda} + \mathbf{f}_{ext}, \quad (4)$$

where $\mathbf{M}$ is the generalized mass matrix

$$\mathbf{M} = \text{diag}(m_1 \mathbb{I}, I_1, \ldots, m_N \mathbb{I}, I_N) \in \mathbb{R}^{6N \times 6N} \quad (5)$$

with $\mathbb{I} = \text{diag}(1,1,1) \in \mathbb{R}^{3 \times 3}$, $m_i$ being the mass and $I_i \in \mathbb{R}^{3 \times 3}$ the moment of inertia of the $i$-th particle.

Further, $\ddot{\mathbf{u}} \in \mathbb{R}^{6N}$ is the generalized velocity vector including linear and angular velocities. The last term in equation (4) represents the external forces and reads

$$\mathbf{f}_{ext} = (\bar{F}_1^T \bar{D}_1 \dot{\lambda}_1 \ldots \bar{F}_N^T \bar{D}_N \dot{\lambda}_N)^T \in \mathbb{R}^{6N} \quad (6)$$

which includes the linear forces $\bar{F}_i$ and the external torque $\bar{D}_i$, both with respect to the center of mass of particle $i$. As regards the first term on the right hand side of equation (4), $\dot{\lambda}_i$ is a Lagrangian multiplier and $\mathbf{J}$ the Jacobi matrix. The latter describes the constrains on the motion of a particle resulting from the contact with other particles. The resulting constrain forces are $\mathbf{J}^T \lambda$.

Using an explicit Euler scheme predicts the new velocity at the next time-step ($\Delta t$, superscript $t + 1$) as $[11]$

$$\ddot{\mathbf{u}}^{t+1} = \ddot{\mathbf{u}}^t + \mathbf{M}^{-1} \mathbf{J}^T \Delta t \lambda + \Delta t \mathbf{M}^{-1} \mathbf{f}_{ext}^t. \quad (7)$$

To solve this equation it is crucial to determine the constraints accurately by building the matrix

$$\mathbf{J} = \begin{bmatrix} \mathbf{J}_{row1}^T & \mathbf{J}_{row2}^T & \mathbf{J}_{row3}^T \end{bmatrix}^T \in \mathbb{R}^{3 \times 12}. \quad (8)$$

The matrix $\mathbf{J}$ consists of three rows, the first one avoids particles to penetrate each other, the following two rows represent Coulomb’s friction in two spatial directions.
3. Results

We present tests of the new algorithm regarding the time evolution of multiple particles. In all cases discussed in the following $8^3$ particles are initially distributed equally spaced within a cubical box of a side length of 8 cm as visualized in figure 1. Figure 1(a) and (b) are a side view where the gravitational vector points downwards and (a) and (b) depict a view from the top on the box, i.e. the gravitational vector points towards the visualization plane. The particles are colored according to their initial position to give an impression of the mixing inside the box. All particles are of a diameter of 2 mm and an initial velocity magnitude of 0.5 m/s. The direction of the initial vector is chosen randomly for each particle. Further, the particles are of a material density of 4000 kg/m$^3$.

More specifically, in the case in figure 1(a)-(c) the particles are uncharged, of a restitution coefficient of $e = 0.3$, and van der Waals forces are considered. The time evolution of the particle locations was computed using the new algorithm. In the side view it can be observed that the particles initially evolve randomly. However, already at $t = 0.03$ s (not shown) the particle density in the upper section is reduced due to gravitational acceleration downwards. Thereupon most kinetic energy is destroyed once the particles collide with the bottom boundary of the box and, therefore, the particles settle fast. After $t = 0.1$ s most particles are located in the bottom section of the box and after $t = 0.28$ s the particles form a single layer and only few particles are still airborne.

In the view from the top on the box (c) one can ascertain how the particles tend to migrate towards the box side walls. This apparent migration is also linked to the destruction of energy during collisions. Once the particles contacted the walls they are reflected with a reduced velocity and, thus, remain in the vicinity of the boundaries. However, most interesting is the formation of structures consisting of several particles which are clearly visible in the top view at $t = 0.28$ s. These structures are the longest and most complex in the regions of the box corners and less pronounced in the center of the box where less particles are present.

In figure 2 the occurrence of these structures depending on the presence of different forces and the chosen algorithm is further elaborated. The figures depict the pdf of the distance of each particle to their next closest neighbor particle at a certain state of the system. In particular, the green curve in figure 2(a) corresponds to the state shown in figures 1(b) and 1(c). This curve exhibits a distinct peak where the ratio of the particle spacing and size equals unity, i.e. the vast majority of particles are in direct contact with another particle. In other words, most particles are part of an agglomeration which confirms the above findings. If van der Waals forces are not considered (blue and red curves in figure 2(a)) this peak substantially attenuates. The instantaneous particle positions for this condition are plotted in figure 1(d). This snapshot ascertains that the attenuation of the peak is related to the fact that agglomerations do not form without van der Waals forces which is an expected result confirmed by our simulations.

Whereas the red curve in figure 2(a) was established using the new algorithm, the blue curve stems from the standard implementation. Here, the term standard implementation relates to the common Lagrangian tracking of particles under the influence of various forces, as done in the studies discussed in the introduction, without the consequent consideration of constraint forces. When comparing the results obtained from the new and the standard algorithm it is noticed that, despite their similarity, a peculiar difference is the behavior for particles spacings smaller than their own size. While the pdf corresponding

![Figure 1.](image1.png)

Figure 1. Time evolution of the release of $8^3$ particles of a restitution factor of $e = 0.3$ in a cubical box, (a) and (b) are side views and (c) and (d) are top views. (a)-(c) are computed with the new algorithm including van der Waals forces, (d) with the standard algorithm without van der Waals forces.
Figure 2. Spacing of each particle in the system to the next closest particle, (a) computed with the standard and the new algorithm, with gravitational and with or without van der Waals forces and (d) additionally electrostatic forces.

to the new approach drops to zero, the standard approach predicts values larger than zero. The reason for that is revealed observing carefully the individual particles in figure 1(d) which was generated using the standard algorithm. In this snapshot several particles overlap with each other which is largely prohibited by the constrained forced acting in the new algorithm. These constraint forces effectuate that the particle spacing is lower bounded by the particle size, which is a clear advantage of our new approach compared to standard approaches. It is noted that overlapping can also be prevented by the standard approach but due to the statically overdetermined state of an agglomeration this comes at high computational costs.

Finally, in figure 2(b) particles under the influence of electric charges, whereas van der Waals forces are retained, are presented. Each particle in a simulations is assigned a high charge of 1 nC. The red curve corresponds to a case where each particle is charged with an equal polarity whereas the black curve is extracted from a simulation where half of the particles are of the opposite polarity than the other half. Since charges of the same polarity repel each other the particles in form a layer at the walls which affects the appearance of a distinct peak in figure 2(b). In the simulation comprising charges of opposite polarity the layer formation is prevented. Instead, the sticking of particle couples of opposite polarity is suggested. However, it is noted that these results represent rather a confirmation of the capability of our algorithm than a portray of a physically exact state since the considered charges are very high and the important mechanism of orientation of dipoles due to induced charges is not considered.

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