

Lagrangian model for predicting the dynamic behavior of cohesive particles in a fluidized confined environment

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Abstract: Titanium dioxide, TiO_2 , is one of the most important raw materials in the paint production process; also TiO_2 is classified as a Geldart C solid type, and it makes its storage and handling more than important not only because of its importance to the process but also because of its complicated nature. Most common problems encountered handling and storing TiO_2 come from the cohesive nature of the solid, which benefits the formation of agglomerates leading to clogging in pipes and storage vessels. Attempting to simulate TiO_2 's handling and storage, a Lagrangian particle simulation began by using a Discrete Element Model. Understanding the interactions and forces acting on solids when they are dispersed in a gas and then stored, and the agglomerate formation due to cohesive forces were the main purposes of this work. The particle motion under the influence of gravity and a fluid in motion was simulated with the BBO equation for each of the particles. The wall-particle collisions were simulated with the equations for exchange of momentum and energy; the particle-particle collisions were simulated with the hard sphere model using as well the equations for exchange of momentum and energy and the agglomerate formation considered the collision model and a cohesion parameter. Three hypotheses were proposed for the analysis of the interactions acting on the particles and their behavior was compared with results from various authors to conclude on the final validation of the DEM here proposed.

Keywords: Lagrangian Simulation; Particle interaction; Multiphase flow simulation; Collision; Cohesion; DEM; Titanium dioxide; TiO_2 .

1 INTRODUCTION

In a paint production plant the storage of TiO_2 powder for large periods of time is considered a bottleneck as the powder after days of being stored forms agglomerates that not even the fluidization control cycle can break and it makes the raw material an unproductive big chunk of powder leading to process delays and extra costs. Understanding the forces acting on a cohesive powder and determining the operation conditions for its storage, in terms of time and weight before the agglomerates are too big for the automatic normal process to flow are the interest of this work and for which the numerical method for simulating the process was intended. In the case of transport and storage of fine cohesive powder, the multiphase approach is preferred.

Particle motion simulations in a multiphase flow have been of great interest not only in the academy, but in the industry. Understanding the forces acting between two or more phases in a multiphase flow could help not only the mechanical performance of industrial processes, but their chemical efficiency as well. Many methods have been formulated to simulate this interaction between the phases, some Eulerian, some Lagrangian; each with pros and cons. When the main focus of the investigation are the particles, then the Lagrangian method is preferred, due to its ability to predict the specific behavior of the particles and some properties impossible to follow up in the Eulerian approach. These include low and high stress/strain systems, multiphase assemblies and even reactions and heat transfer [23].

For the purpose of this work, a Discrete Element Method (DEM) with dynamic response of Central Difference method was chosen because in each time step the trajectory and the rotation of each particle due to the relevant forces acting on each particle and the interaction between the particles themselves and their environment are calculated; this way the method proposed could bring, as seen in the references, accurate results of the behavior of cohesive powders after transport [23]. Finally the model can be used not only for understanding the dynamics of the powder particles but also the behavior of the powder after long periods of storage. The main advantage of the DEM Method is that highly complex systems can be modeled with basic data without oversimplifying assumptions and its biggest limitation is the computational time required for large number of particles.[12][13][23][24]

In the literature review there can be found several articles regarding the transport of particles, the accurate method of identifying the probability of particle collisions and their effect on their velocities. Most of the authors only take in consideration one set of interactions, like collisions only with a wall, rebound with one wall, different particles transport methods without interaction (like Eulerian or Lagrangian), fluid velocity component in only one direction, one direction collisions with other particles and constant initial position of the particles [1][2][7][8][10][11][18][19][20].

The present work takes in consideration all of the components of the literature review with the intent of having an accurate method for the simulation of transport and storage of cohesive powder. It proposes a method where wall collisions are taken in consideration due to a confined environment and multiple particle collisions could happen in a small time step, possibly leading to agglomerate formation. In this paper, not only the drag force affects the dynamic behavior of the particles but the cohesion force as well.

2 MATHEMATICAL MODEL

The next section contains a recapitulation of the equations employed in the model, with a brief definition of each of the terms and the reasons for which each was used.

2.1 Equation for the particle motion, only under the action of external forces without collision

To calculate the velocity of the particles under the action of gravity, and their interaction with a moving fluid, the Basset–Boussinesq–Oseen equation (BBO equation) was used. From this the position of the particles at each instant of time is obtained and this information is used to plot the particle trajectories. The general BBO equation form is illustrated in equation 1 (added mass and basset force are not included). For further understanding of the application of the BBO equation refer to Crowe [12] chapter 4.

$$m \frac{dv_i}{dt} = mg + Vd \left(-\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} \right) + 3\pi\mu_c D \left[(u_i - v_i) + \frac{D^2}{24} \nabla^2 u_i \right], \quad (1)$$

where

g is the gravity,

p is the fluid pressure,

τ_{ij} is the shear stress on the particle due to the fluid,

μ_c is the viscosity of the fluid,

D is the particle diameter,

u_i is the fluid velocity and

V_d is the volume of the particle.

The term on the left contains the change of the particle velocity in time $\left(\frac{dv_i}{dt}\right)$ as the unknown variable and the particle mass (m). The right side of the equation is the extended version of the sum of all the forces acting on the particles as it is stated in Newton's Law of movement. The forces included in

equation 1 are: the gravity effect (mg), the pressure and shear stress from the fluid $\left(-\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j}\right)$ and the steady state drag $\left(3\pi\mu_c D \left[(u_i - v_i) + \frac{D^2}{24} \nabla^2 u_i\right]\right)$. On this side of the equation it can be added any other forces that may be acting on the particle and that may be intended for analysis, like the cohesion force (this term is not included in the equation (1, to show the BBO equation in its pure essence due only to illustrative reasons).

2.2 Collision detection

For the collision detection between two particles at each time step, a cycle starts where a particle is chosen as reference and for which the position of its center is measured against the centers' positions of each of the rest of the particles of the system and then compared to a minimum contact distance set at a value equal to the sum of the particles radius to avoid superposition. If the distance between a set of two particles is less than the minimum contact distance then there is a collision, and the post-collisional velocities and particles position must be calculated with the method described in the next section.

For the case of the particle-wall collision detection at the time step considered, each particle center's position is compared to the coordinates of the confined system and if the position of the particle exceeds the coordinates of the system then there should have been a collision and hence the particle position is corrected to a position no further than the confined environment coordinates and then the post-collisional velocities and particles positions are calculated.

2.3 Collision-cohesion forces

The problem of particle-wall and particle-particle collisions is frequently found in the storage of solids, the pneumatic transport, and flow and clogging of pipes, channel flows, fluidized beds and many more; making it a subject of high interest in the industry not only for the operations efficiency but for the process productivity. The treatment of the mechanical behavior associated with particle-wall and particle-particle collisions depends on the inertia of the particle, when a collision takes place and there is a rebound, a loss of kinetic energy due to friction and inelasticity effects can be observed. [12]

For simulating any type of collision, either the soft sphere or the hard sphere model can be used; this work employs the hard sphere because of its ability to rapidly integrate the post-collision velocities of the particles with the BBO equation for a given time step, allowing space to direct the attention to the real focus of this work: the cohesion force.

The simulation of the hard sphere model considers momentum difference of the particles for a binary collision either against a wall or another particle. The considered model has its basis in two simple equations for one particle, but it needs to be expressed for the n-particles with which there has been a collision with the correct velocity direction signs and conventions considering the pre and post-collision states. [8][9][10][11][12]

$$m(\mathbf{v}^{(1)} - \mathbf{v}^{(0)}) = J \quad (2)$$

$$I(\boldsymbol{\Omega}^{(1)} - \boldsymbol{\Omega}^{(0)}) = -\mathbf{r} \times J \quad (3)$$

In equations 2 and 3, the term of the right is the impulse force due to collision (J); m and I are the mass and moment of inertia of the particle, finally v and Ω are the translational and rotational velocities of the particle, where the superscripts (1) and (0) refer to the pre (0) and post collisional (1) states of only one particle. [8] [9] [10] [11] [12]

Considering the case where the particles continue sliding after collision, the equations for the post-collision velocities of one particle are:

$$\mathbf{v}_1 = \mathbf{v}_1^{(0)} + \frac{J_{n,c}}{m_1}(\mathbf{n} - f\mathbf{t}) - \frac{m_2}{m_1 + m_2}(1 + e)\mathbf{n} \cdot \mathbf{G}^{(0)}(\mathbf{n} + f\mathbf{t}) \quad (4)$$

$$\mathbf{v}_2 = \mathbf{v}_2^{(0)} - \frac{J_{n,c}}{m_2}(\mathbf{n} - f\mathbf{t}) + \frac{m_1}{m_1 + m_2}(1 + e)\mathbf{n} \cdot \mathbf{G}^{(0)}(\mathbf{n} + f\mathbf{t}) \quad (5)$$

$$\boldsymbol{\omega}_1 = \boldsymbol{\omega}_1^{(0)} + \frac{5}{2r_1}(\mathbf{n} \times \mathbf{t})f \left[-\frac{J_{n,c}}{m_1} - \frac{m_2}{m_1 + m_2}(1 + e)\mathbf{n} \cdot \mathbf{G}^{(0)} \right] \quad (6)$$

$$\boldsymbol{\omega}_2 = \boldsymbol{\omega}_2^{(0)} + \frac{5}{2r_2}(\mathbf{n} \times \mathbf{t})f \left[-\frac{J_{n,c}}{m_2} - \frac{m_1}{m_1 + m_2}(1 + e)\mathbf{n} \cdot \mathbf{G}^{(0)} \right] \quad (7)$$

The subscripts in the J term refer to the normal and tangential components of the impulse and are calculated as follows and according to the model proposed by Kosinski and Hoffman [8][9][10]:

The normal impulse is calculated from the sum of the adhesion and cohesion normal impulses of the particles after a collision.

$$J_n = J_{n,a} + J_{n,c} \quad (8)$$

Both the $J_{n,a}$ and the $J_{n,c}$ are considered for the case where the particles continue sliding after collision.

$$J_{n,a} = -\frac{m_1 m_2}{m_1 + m_2} (1 + e) (\mathbf{n} \cdot \mathbf{G}^{(0)}) \quad (9)$$

$$J_{n,c} = \int_0^{t_c} F_{n,c} dt = 0.238 \left(\frac{m^2}{E_*^2 (\mathbf{n} \cdot \mathbf{G}^{(0)})} \right)^{1/5} \frac{Ar^{4/5}}{D_c^2} \quad (10)$$

In equations 4-7 and 9-10, \mathbf{n} represents the normal vector of the surfaces that are in contact in the collision process, $\mathbf{G}^{(0)}$ is the relative velocity between the particles centers after collision; when the collision is with a wall, the same equations can be considered but taking note that only particle is active in the collision process; e is the restitution coefficient of the powder considered, for this case problem a value of 0.9 is used; A is the Hamaker constant, r is the particles radius in m, D_c is the particles spacing between contact and it is set at a value of 0.02 nm [10] and lastly E_* is the effective Young's Module [10]. Equations 4-10 calculate the particle velocities after there is a collision, reinforcing the fact that the cohesion force only acts when there is contact between the particles.

2.4 Consideration for agglomeration due to collisions and the action of the cohesive force

After collision between two particles has taken place, normally the post-collisional velocities of each particle must be calculated; but in the case where cohesion force is considered, an additional dimensionless parameter β should be contemplated. This parameter is used for the definition of the formation of agglomerates or the repulsion between the particles after the collision [29].

In order to simplify the modeling of the agglomeration parameter β , a Φ term is considered which includes the diameters of two agglomerates or particles in the time step of the collision.

$$\Phi = \frac{d_{a1}}{d_{a2}} \quad (11)$$

In an instant collision between two particles, assuming they form an agglomerate, following the mathematical development of the forces acting on agglomerates by Zhou and Li [29], the parameter β is calculated as follows.

$$\beta = \frac{\frac{A(\rho_a - \rho_f)g}{\pi \delta^2} \frac{2\Phi}{1+\Phi}}{\left[\frac{0.996(\pi v^6 \rho_a^3)}{\pi k^2} \right]^{1/5} \left(\frac{2^4 \Phi^{10}}{(1+\Phi)^3 (1+\Phi)} \right)^{1/5}} \quad (12)$$

For the case of this model, β is considered as the valid criteria for agglomeration formation or not, with the following considerations:

- $\beta \leq 1$, two particles or agglomerates separate after collision; agglomerate breaks.

- $\beta > 1$, two particles or agglomerates coalesce after collision; agglomerate is form.

After the agglomeration factor has been applied and if an agglomerate will be formed, then properties such as mass, density, translational and rotational velocities of the agglomerate, with the equations presented by Kosinski & Hoffmann, are calculated to integrate the agglomerates in the particles' movement and drag by the air [9][10]. Eq. 13 calculates the velocity through the conservation of momentum of the particles that formed the agglomerate.

$$m_1 v_1^{(0)} + m_2 v_2^{(0)} = (m_1 + m_2) v_{agg} \quad (13)$$

3 MODEL APPLICATION AND ALGORITHM

Once the equations needed to describe the phenomena of the problem are considered, they are integrated in an algorithm and later programming in Matlab in order to being able to simulate specific cases and compare the results obtained of particles' trajectories and velocities with data from the references.

The algorithm programmed is capable of simulating n particles in random initial positions in a confined environment and submitted to an air current with constant velocity (v_f). At the beginning of the simulation both the particles and the air current are at rest and as soon the algorithm initiates the time integration, the particles velocities and position are calculated validating if they are in contact with each other, with the wall or only interacting with the air flow. Depending on each case valid in the time step considered, the algorithm uses different equations and parameters.

The easiest case is where the particle interacts only with the air current and there are no collisions with other particles or with any wall of the closed environment. For this case, as a predictor for the particles velocities the equation (1) in the central difference method form is employed.

For the case where the particle collides with the wall the equations considered in section 2.3 are used, with the special consideration where the velocities of a second particle are set to 0 and there is no cohesion or adhesion force.

Lastly, for the case where there are collisions between particles or agglomerates as particles and cohesion takes place, the hard sphere model is considered applying the equations described in section 2.3.

For the case where the agglomeration is formed, the model proposed by Zhou and Li in [29] and illustrated in section 2.4 is used. The first agglomeration formation begins with the collision of two

particles and the interaction of the cohesion force and the consideration of the agglomeration parameter. When the agglomeration parameter concludes with the agglomeration of the two particles colliding then a new particle is formed, with a new mass, particle diameter and density; after the new particle is created the algorithm programmed calculates the post-collision velocities and agglomerates position to restart with a new time step.

4 MODEL VALIDATION

As a validation protocol of the method and algorithm's accuracy, several simulations were made using particles with different diameters, densities and under the influence of a fluid with different velocities and directions [24]; three hypotheses were formulated, and for each tests were conducted to prove the accuracy and consistent behavior of the particles under the influence of airflow and the effects of various phenomena during the simulation, like cohesion, collision among particles and against the walls.

4.1 Hypothesis 1: The model is capable of identifying the forces that act on the particles for a given time step.

The forces acting on a particle that is being transported by a moving fluid in a simplified point of view are: Drag, Gravity and Damping. For the special case of this hypothesis, only the normal damping force, on a regular powder, was proven in a 3 second period, with a 0.1 second time step, three simulations were conducted for one particle free fall; the standard model was individually modified different initial y-positions (1.8, 1.4, 1 m) in a 2x2 m confined environment and with a densities ratio equal to $\rho_p = 1.6\rho_g$. Fig 1 shows normal damping force for the three simulations, changing the initial height of the particles.

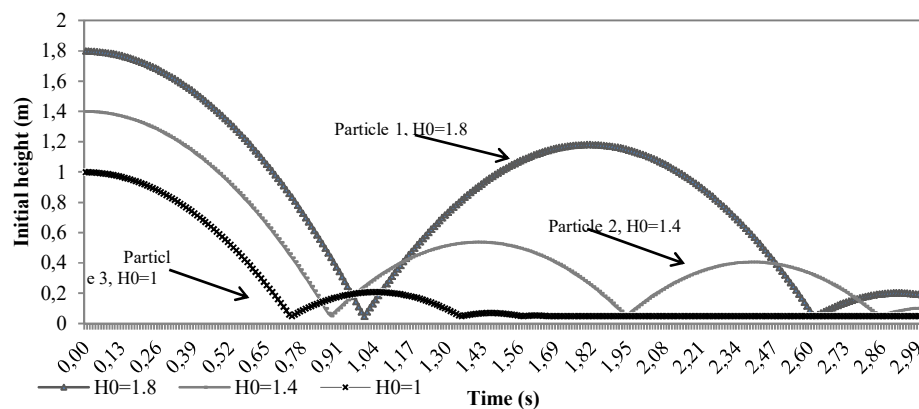


Figure 1. Normal damping force at three different initial heights

Fig 1 shows the particle's position (height) in time for three different initial positions until it hits the lower base of the confined environment and trying to make it back to its initial position, but with the balance of gravity, collision repulse and air drag, it fails to reaching the initial height; as time passes each time the particle bounces up and down the particle loses momentum until it reaches the equilibrium at the bottom of the domain. It is easy to visualize in Fig 1, how the higher the height the longer the time to hit the ground (case, particle 1 where $H_0=1.8$ m) and the longer time until it reaches the equilibrium at the base of the confined environment. Taking in consideration Fig 1 and the concepts by Choi et al [24], the hypothesis 1 is proven right and it can be said that the model here formulated does identify the forces acting on the particle and the effect that they have on its trajectory.

4.2 Hypothesis 2: The particle-wall collisions affect the trajectory of the particle's transport

To identify the effect of wall-particle collisions, a simulation was run for 10 particles with random initial position, a 0.02, 0.03 and 0.04 m particle diameter and air velocity of 0.002 m/s in the x direction. Fig 2, 3, 4, shows the effect of the collisions on the particles trajectories; when the particle collides with a lateral wall, the particle shows a trajectory inverse to the one it hit the wall with, in the case of this simulation when the particle hits the lateral wall the x velocity of the particle becomes negative. When the particle hits the bottom wall, the damping effect acts again until it reaches equilibrium. Also in Fig 2,3,4, as explained by Sommerfeld and Kussin [26] it can be seen how the effect of the particle diameter affects the outcome of the collision; that is, the bigger the particle diameter the bigger the effect on the instant particle trajectory due to wall collisions and the faster the particles reaches equilibrium.

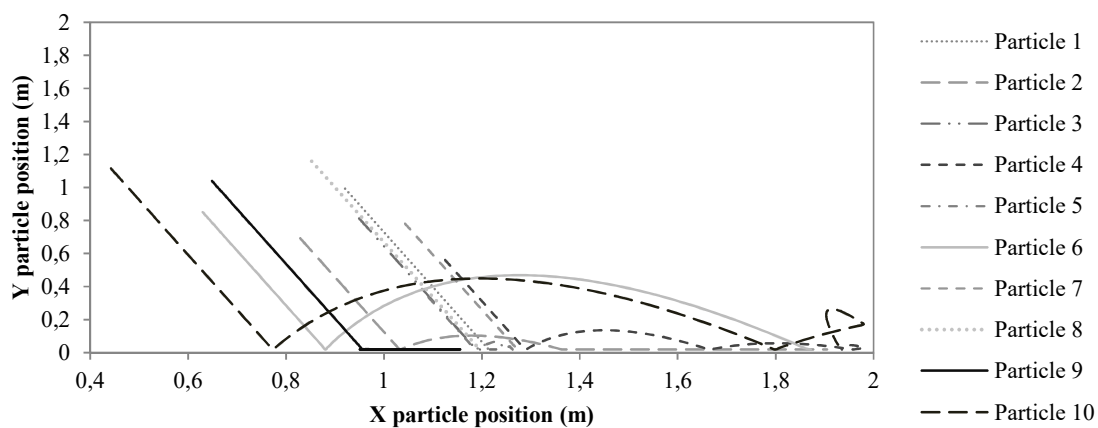


Figure 2. 0.04 m particle diameter trajectories with wall collisions

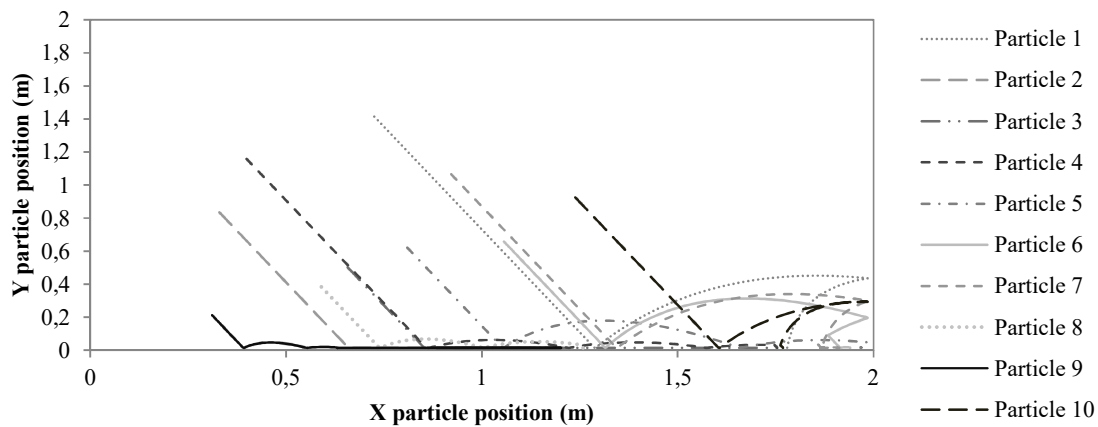


Figure 3. 0.03 m particle diameter trajectories with wall collisions

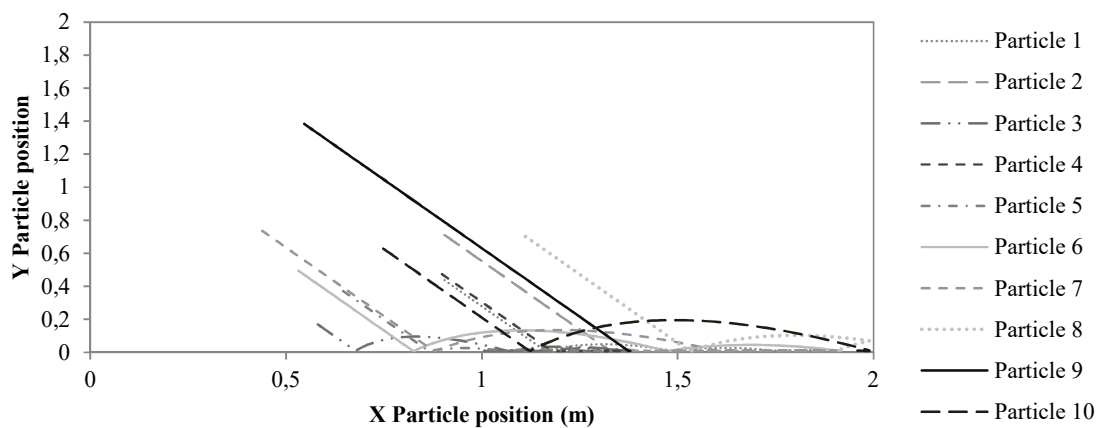


Figure 4. 0.02 m particle diameter trajectories with wall collisions

4.3 Hypothesis 3: Particle-particle collisions and interparticle cohesion force affect the velocity of the particles

One of the principal concerns of analyzing the cohesion force after a collision or contact is the agglomeration formation and hence the reduction of the individual particle velocities; in a fluidization process the significant reduction of the particles velocities and weight increase translates in an extra effort from the air current to fluidize the powders, sometimes the reduction in the particles momentum is so big that the fluidization reaches a point that even with an air current, the powder does not move. The model must be able to predict the possibility and frequency of this phenomenon in order to consistently predict the behavior of the powder after large storing times.

To visualize the effect of the particle-particle collisions a simulation with 10 particles was run, a ratio of particle position (y) and total height of the confined environment (H) equal to 0.01 ($y/H= 0.01$) was chosen [20]. This ratio considers a high concentration of particles in the confined environment leading to a

high probability of collisions so it can be visualized its effect on the particles velocities. Fig 5, shows the model particles x velocity direction distribution with the effect of the collision frequency; it can be examined how with at an average particle velocity of 0.5 m/s and a high frequency of collisions the particles velocities are affected with a 95% of confidence by a standard deviation of 0.32. Concluding that, with no agglomeration formation, at higher frequencies of collisions the higher the velocity of the particles.

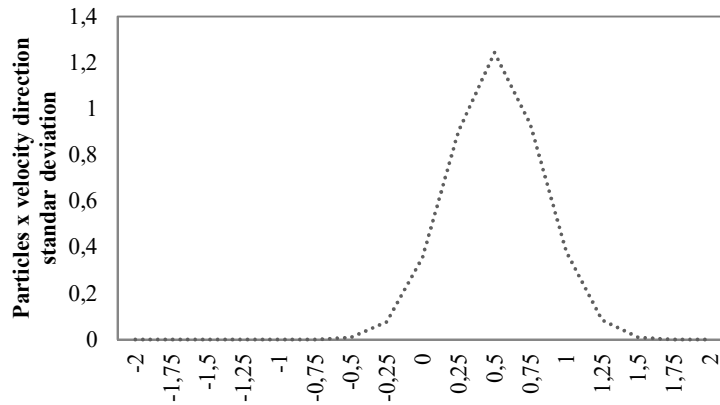


Fig 5. Velocity distribution vs. Collision frequency

To understand the influence of the cohesion force on the particles, fig 6 shows how after a contact between particles the cohesion forces starts being considered in the equation of movement, to finally affect the velocity of the particles. Fig 6, illustrates the quantification of the cohesion force of one particle in a 10 particle system that collided in a 2 seconds simulation with a 0.5 time step, and how as soon as the first impact takes place the cohesion force appears and by its negative value it will affect the velocity of the particle and possible will contribute to the formation of an agglomerate.

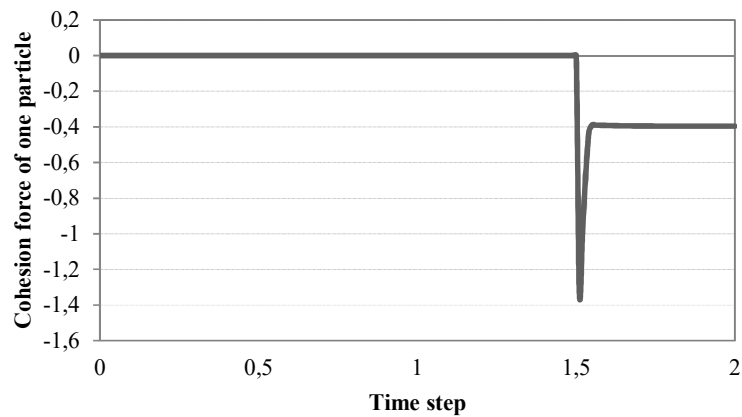


Figure 6. Quantification of the cohesion force in a collision

Finally, to evaluate the agglomerate formation, the data found that could be compared are snapshots of the particles and agglomerates positions in a point of time and the accumulated number particle-particle collisions and the ones resulting in agglomerates formation [10].

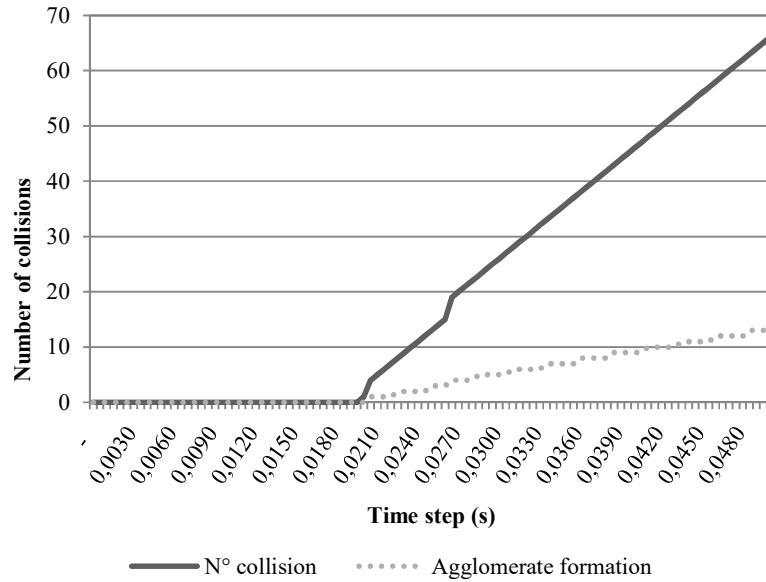


Fig 7. Accumulated number of collisions and agglomeration formation

In Fig. 7, it can be observed how, in a n particles simulation with the application of the β parameter not all the collisions generate an agglomerate and there is a correlation of 1:4 between the accumulated number of collisions occurring in a time step and the number of agglomerates created in each collision. These findings are consistent with the finding presented by Kosinski and Hoffman [10].

5 CONCLUSIONS

Although this model has a focus on the storage and handling of TiO₂, it sets a basis for the continuation of particle simulation with as many restraints as the solid has, besides cohesion. This model can be used for the simulation of gas-solid separators, pneumatic transport and many other process applications where multiphase flows are being considered with the adjustment of the geometry of the domain, the inclusion of the fluid-wall interaction and the final assembly of the particle phase and the fluid phase.

Finally, after validating the ability of the model proposed in this work to predict the behavior and dynamics of particles being submitted to an air current including collisions between particles and with the walls, taking in consideration the cohesion force and the formation of agglomerates, following work

should be to set a laboratory experiment to compare the algorithm results with real time data so the model can be extrapolated to the problem of the TiO₂ which originated this work.

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