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Numerical study of agglomeration modeling in polydispersed gas-solid flows with respect to particle separation

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ABSTRACT

In this paper the numerical particulate flow model EUgran+Poly (Schellander et.al, 2012b), which is an Eulerian-Lagrangian and Eulerian-Eulerian numerical hybrid model for dilute and dense rapid granular flows, is modified to account for agglomeration. We introduce a novel approach referred as, "Bus-Stop Model", where agglomeration is modelled using Lagrangian tracer trajectories. To achieve this goal, two possible agglomeration models are presented: 1) a simple volume balance model, 2) a new implementation of the population balance model by Smoluchowski (Smoluchowski, 1917).

The validation of the new implementation of the agglomeration model is done by comparison with the discretized population balance model, for a simple case. Furthermore the applicability of the model is shown for an industrial cyclone. The agglomeration model shows the mean particle diameter increases in the cyclone. The simulation results indicate improved quality and accuracy.

NOMENCLATURE

a	characteristic length
c	particle class volume fraction
C	Cunningham slip factor
d	particle diameter
g	gas phase
G	volume agglomeration rate
H	sticking probability
K	agglomeration rate
n	number of particles
p	pressure or particle phase
q	fluid and solid phase
s	solid phase
t	time
T	temperature
V	volume
$\mathbf{f}$	force per mass
$\mathbf{g}$	gravity
$\mathbf{T}$	gas stress tensor
$\mathbf{S}$	solids stress tensor
$\mathbf{u}$	velocity
α	volume fraction
β	drag coefficient, collisional-agglomeration rate
ε	turbulent dissipation rate
η	collision probability
ρ	density
τ	particle relaxation time
μ	dynamic viscosity
ω	relative particle velocity

INTRODUCTION

In chemical industry, pneumatic conveying and separation of solids, particles and dust by fluid based on centrifugal forces and agglomeration processes is very important. Since Smoluchowski (1917) presented his population balance model for particle agglomeration, agglomeration modelling has featured in granular simulations, especially in the chemical and energy industry. The population model with the main agglomeration rate based on collisions and sticking probabilities.

EUGRAN+POLY

The EUgran+Poly (Schellander et.al., 2012a) is a numerical model for the simulation of gas and fluid flows, including particle transport or particle separation. The main idea of EUgran+Poly is to use a hybrid model, which uses parts of the two state of the art models for particulate transport simulation. The two standard models are the Eulerian-Eulerian granular phase model and the Eulerian-Lagrangian discrete phase model. Both models have their advantages and disadvantages, but with a combination of both models, a hybrid model can be created, which uses all the advantages.

Eulerian-Eulerian granular phase

The Eulerian-Eulerian granular phase model, describes the granular material, as a continuum, that is

$$\frac{\partial}{\partial t}\left(\alpha_q \rho_q\right) + \nabla \cdot \left(\alpha_q \rho_q \mathbf{u}_q\right) = 0\,,$$

$$\begin{aligned}\frac{\partial}{\partial t}\left(\alpha_g \rho_g \mathbf{u}_g\right) + \nabla \cdot \left(\alpha_g \rho_g \mathbf{u}_g \mathbf{u}_g\right) = \\ -\alpha_g \nabla p - \nabla \cdot \alpha_g \mathbf{T}_g + \alpha_g \rho_g \mathbf{g} - \beta_s \left(\mathbf{u}_g - \mathbf{u}_s\right),\end{aligned} \quad (1)$$

$$\begin{aligned}\frac{\partial}{\partial t}\left(\alpha_s \rho_s \mathbf{u}_s\right) + \nabla \cdot \left(\alpha_s \rho_s \mathbf{u}_s \mathbf{u}_s\right) = \\ -\alpha_s \nabla p - \nabla \cdot \mathbf{S} + \alpha_s \rho_s \mathbf{g} + \beta_s \left(\mathbf{u}_g - \mathbf{u}_s\right) + \mathbf{f}_{s,add}\,,\end{aligned}$$

The inter-particle collisions are included by kinetic theory closure for the particle stresses, which requires additional pseudo-thermal energy (granular temperature) to describe the energy fluctuations of the particles.

Eulerian-Lagrangian discrete phase

In this model, the forces on one particle are calculated and the particle is tracked through the simulation geometry. In this approach particle specific physical effects, like the Magnus force or rough wall handling for particle wall

collisions can be done. The force balance for one particle is defined with

$$\frac{\partial}{\partial t}\mathbf{u}_p = \beta_p\left(\mathbf{u}_g - \mathbf{u}_p\right) + \mathbf{g} + \mathbf{f}_{magnus} + \mathbf{f}_{p,add}. \quad (2)$$

A disadvantage of this model is, that for each particle the equation must be solved, and if there is a particle-particle interaction included, the search for the collision partners is extremely time consuming. If a huge amount of small particles (e.g. 1 µm particles) is present, this model is inadequate.

Drag model and force transfer between the models

In Schellander et al. (2012b) the usage of the EUgran+Poly model for polydisperse granular materials is presented. Important for the hybrid model is, that both numerical models use the same drag model (Wen and Yu, 1966) for the particles. Forces which are calculated in one approach must be transferred to the other approach, where they are included as additional forces $\mathbf{f}_{add}$. The transfer function is written as,

$$\mathbf{f}_{s,add} = \alpha_s \rho_s \left\langle \mathbf{f}_{p,add} \right\rangle. \quad (3)$$

Usage and calculation procedure

The simulation is based on Eulerian granular approach, which uses additional forces coming from the Eulerian-Lagrangian tracer trajectories. These tracer particles, are computed at fixed times, thus the Eulerian-Eulerian simulation is stopped and on the stationary velocity and volume fraction fields, the tracer trajectories are evaluated. It is important to use enough tracer particles to obtain a smooth force exchange field. Then the simulation is continued.

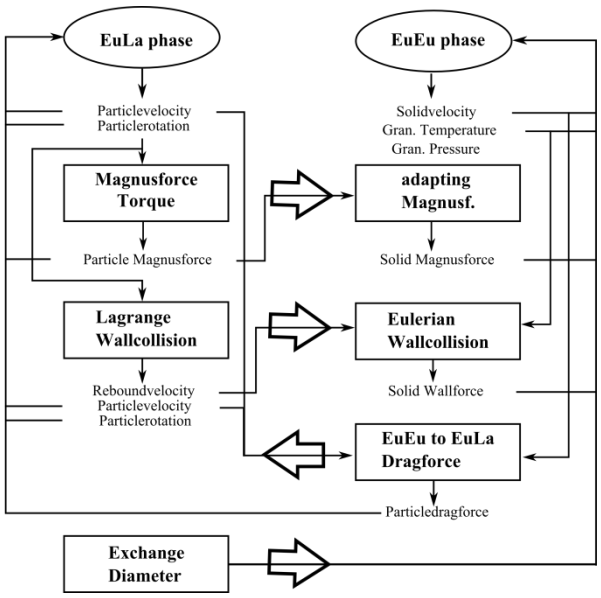

Figure 1: Schematic diagram of EUgran+Poly, (Schellander et. al., 2012b)

AGGLOMERATION

In this section two models for particle agglomeration are presented: 1) the population balance model, 2) the volume balance model. If the particle size distribution for the agglomerated particle cluster and the de-agglomerated particles is known, a simple volume based model, with fixed volume agglomeration rates can be used for computing agglomeration. For a full simulation of agglomeration, the population balance model with computed agglomeration rates should be preferred.

Agglomeration based on population balance

Smoluchowski (1917) presented a population balance model, which describes the particle count of each particle class (*i*) at any time *t*. Agglomeration rates $K(i,j)$ and $K_{i,j}$ based on binary collisions between particles give the rate of agglomeration. These agglomeration rates are based on Brownian-, turbulent-, shear and kinematic collisions, which are discussed later in this section in detail.

The equation for the *i*-th particle population is written as

$$\frac{\partial n(i,t)}{\partial t} = \frac{1}{2}\int_0^i K(l, i-l)n(i-l,t)n(l,t)dl - n(i,t)\int_0^\infty K(i,l)n(l,t)dl \quad (4)$$

with $n(i,t)$ as particle count in class *i* at time *t*. For usage in computational fluid dynamic simulation the equation must be discretized yielding

$$\frac{\partial n_i(t)}{\partial t} = \frac{1}{2}\sum_{j=1}^{i-1} K_{i-j,j}n_{i-j}(t)n_j(t) - n_i(t)\sum_{j=1}^{\infty} K_{i,j}n_j(t). \quad (5)$$

In a simulation it is not possible to use an infinite number of particle classes, therefore a maximum number *N* of particle classes must be chosen. Recognizing that the highest particle class cannot lose any particles to higher classes, the equation system is finally written as

$$\frac{\partial n_i(t)}{\partial t} = \frac{1}{2}\sum_{j=1}^{i-1} K_{i-j,j}n_{i-j}(t)n_j(t) - n_i(t)\sum_{j=1}^{N} K_{i,j}n_j(t). \quad i < N \quad (6)$$

$$\frac{\partial n_i(t)}{\partial t} = \frac{1}{2}\sum_{j=1}^{i-1} K_{i-j,j}n_{i-j}(t)n_j(t) \quad . \quad i = N$$

Agglomeration rates

The agglomeration rates are calculated based on Brownian-, turbulent-, shear and kinematic collisions (Park et al., 2002). In detail, the agglomeration rate is written as (Anh, 2004)

$$K_{i,j} = \eta_{i,j}\beta_{i,j}H_{i,j}, \quad (7)$$

where $H_{i,j}$ denotes the sticking probability, $\eta_{i,j}$ is the collision probability, describing the reduction of the collision rate by the surrounding fluid and $\beta_{i,j}$ is the collision-agglomeration rate for the particles *i* and *j*. The values for the sticking and hitting probability are between 0 and 1, which is discussed by Anh (2004), and literature

cited therein, for simplicity in this paper both are chosen with 1.

Brownian motion

The model for describing the Brownian collision rate depends on the Knudsen number (Nowakowski and Sitarksi, 1981). In this paper, where the Knudsen number is much less than 1 (continuum regime) the following equation can be used,

$$\beta_{i,j} = \frac{2kT}{3\mu}\left(\frac{1}{d_i} + \frac{1}{d_j}\right)\left(d_i + d_j\right), \tag{8}$$

where k denotes the Boltzmann constant.

Turbulence

The turbulent agglomeration can be divided into two parts, the turbulent shear gradient part and the turbulent acceleration part, written as

$$\beta_{i,j} = \sqrt{\frac{8\pi}{3}}\left(\frac{d_i}{2} + \frac{d_j}{2}\right)^2 \sqrt{\omega_a^2 + \omega_s^2}\,, \tag{9}$$

with ω as relative particle velocity. Saffman and Turner (1956) derived a collision kernel which combines the shear and acceleration mechanism.

$$\beta_{i,j} = \sqrt{\frac{8\pi}{3}}\left(\frac{d_i}{2} + \frac{d_j}{2}\right)^2 \left[3\left(1 - \frac{\rho_f}{\rho_p}\right)^2 \times \left(\tau_i - \tau_j\right)^2 \left(1.16\sqrt{\frac{\varepsilon^3}{\upsilon}}\right) + \frac{1}{5}\left(\frac{d_i}{2} + \frac{d_j}{2}\right)^2 \frac{\varepsilon}{\upsilon}\right] \tag{10}$$

τ_i denotes the particle relaxation time and is defined as (Park et al., 2002)

$$\tau_i = \frac{C_{c,i}\left(2\rho_p + \rho_f\right)d_i}{36\mu}, \tag{11}$$

with $C_{c,i}$ as Cunningham slip correction factor, which is in our case close to 1. Kruis and Kuster (1997) presented modified derivations of ω_a and ω_s, which are thoroughly reviewed and discussed by Park (2002). In the work of Kruis and Kusters (1997), the relative velocity based on acceleration and shear is represented with the following two equations:

$$\omega_a^2 = 3\left(1-\delta\right)^2 v_f^2 \frac{\chi}{\chi - 1} \times \frac{\left(St_i + St_j\right)^2 - 4St_i St_j \sqrt{\frac{1 + St_i + St_j}{\left(1+St_i\right)\left(1+St_j\right)}}}{St_i + St_j} \times \left\{\frac{1}{\left(1+St_i\right)\left(1+St_j\right)} - \frac{1}{\left(1+\chi St_i\right)\left(1+\chi St_j\right)}\right\} \tag{12}$$

and

$$\omega_s^2 = 0.238\delta v_f^2\left(\frac{St_i v_i^2}{C_{c,i} v_f^2} + \frac{St_j v_j^2}{C_{c,j} v_f^2} + 2\frac{\overline{v_i v_j}}{v_f^2}\sqrt{\frac{St_i St_j}{C_{c,i} C_{c,j}}}\right) \tag{13}$$

with v_f, v_i and v_j as root mean square velocities and the correlation of velocities $\frac{\overline{v_i v_j}}{v_f^2}$, for which we use the relations proposed by Park et al. (2002). St_i denotes the Stokes number, which is calculated with

$$St_i = \frac{\tau_i}{T_L}, \tag{14}$$

with T_L as Lagrangian time scale (Park et al., 2002).

χ and δ are dummy variables for (Anh, 2004)

$$\delta = \frac{3\rho_f}{2\rho_p + \rho_f} \tag{15}$$

and

$$\chi = 0.183\frac{\sigma_f^2}{\sqrt{\varepsilon\nu}}. \tag{16}$$

In Figure 2 a result for the different effects in the agglomeration rate of a particle $d_i = d_{\mathrm{Ref}} = 1$ µm with particles

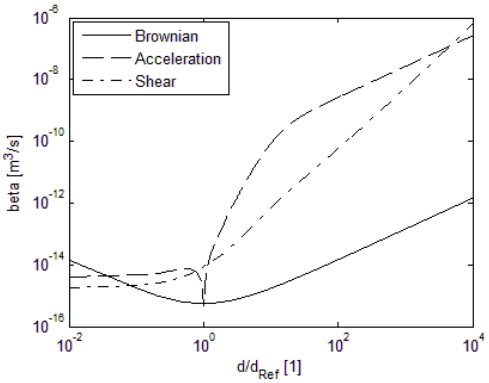

Figure 2: Schematic diagram, showing the agglomeration rate amount of the different effects for a $d_{\mathrm{Ref}} = 1$ µm particle.

$d_j = 0.01$ µm ... 10 mm are shown. It can be observed that for small particles, the Brownian agglomeration effect are nearly same as turbulent effects, with increasing diameter the impact compared to turbulent agglomeration decreases. Hence for particles greater 1 µm the Brownian agglomeration can be neglected.

Particle size distribution

One important question is how to discretize the diameters for the particle classes to comply mass conservation. If two particles, *i* and j , agglomerate the resulting particle should have the volume of the two initial particles. Thus, the following discretization rule must be used for the *i*-th particle class diameter,

$$d_i = i^{\frac{1}{3}} d_{\min} \tag{17}$$

where $d_{\min}$ denotes the minimum diameter in the particle size distribution. In industrial facilities particle size distributions are often present over several orders of magnitude therefore, such a discretization is unfeasible. In literature (Anh, 2004) several solutions for the discretization of the particle diameter are given, but they guarantee only that the error of mass conservation is less than approximately 5 to 10 %. In case of particle separation efficiency studies, an agglomeration model must accurately conserve mass. In the following section we present two different approaches solving this deficiency of the standard discretization of the Smoluchowski equation.

Model application

The first step is to implement the population balance directly. This can easily be realized in a Eulerian granular phase simulation with modelling for each particle diameter class an own granular phase. The problem is, that this is too time consuming, because for each phase the complete equation system, including coupling equations for phase-to-phase interaction, must be solved. Another problem is, as mentioned before, that mass conservation must be guaranteed, which needs 1000 particle classes per diameter decade (17). A simple model which avoids this problem is the volume balance model in the following section.

Volume balance model

The first mass conserving model is based on the idea of reinterpretation of the Smoluchowski equation, using a balance equation system and can be simply implemented The idea is, that not only binary particle collisions are considered, but to model the mass transfer from collisions of particle classes *j* and *v* to class *i*. This can be realized without recognizing any diameter dependencies. A cluster of particles *j* can also combine with a cluster of *v* particles to a particle with diameter *i*. Another assumption for this model is that the final particle size distribution has to be known and the agglomeration rate $G_{i,j,v}$ is assumed to be constant for each particle collision pair *j*,*v*, adding volume to class *i*. The agglomeration rate is zero when the final particle size distribution is reached by a specific particle classes. The equation system can be written as,

$$\begin{aligned}\frac{\partial c_i(t)}{\partial t} V_{cell} = &-\frac{1}{2} c_i(t) \sum_{j=1}^{N-1} \left(\sum_{v}^{N} G_{i,j,v} \right) c_j(t) \\ &+ \sum_{j=1}^{i-1} c_j(t) \left(\sum_{v=1}^{j} G_{i,j,v} c_v(t) \right) \\ &- \frac{1}{2} c_i(t) \left(\sum_{v}^{N} G_{i,i,v} \right) c_i(t) \quad i < N \end{aligned} \tag{18}$$

$$\frac{\partial c_i(t)}{\partial t} V_{cell} = \sum_{j=1}^{i-1} c_j(t) \left(\sum_{v=1}^{j} G_{i,j,v} c_v(t) \right) \quad i = N$$

where c_i denotes the volume fraction of particle class i and V_{cell} the regarded volume. This model is suitable to be used for modelling agglomeration in systems where the initial and the final particle size distributions are known. Neither special particle diameter distribution must be used, nor material parameters of the granular must be known. These are represented by the agglomeration rate $G_{i,j,v}$, which is modelled as a constant. However it is difficult to obtain reasonable values for $G_{i,j,v}$, since no explicit relations exist, though they may be obtained by experiments.

Bus-Stop model

If we discretize the population balance equation by considering Lagrangian trajectories for each particle class, it is possible to compute agglomeration with the Smoluchowski approach with mass conservation. Hence, agglomeration is considered as exchange of mass between trajectories *i* and *j*. Since we use the Smoluchowski equation the proposed equation for the agglomeration rates $K_{i,j}$ can be used directly, in contrast to the Volume balance model.

The Bus-Stop model is sketched in Figure 3. It is divided in 3 subsequent steps.

1.) Computation of tracer trajectories without agglomeration modelling. In each cell, which is hit by a trajectory, the particle velocity and particle number is stored.

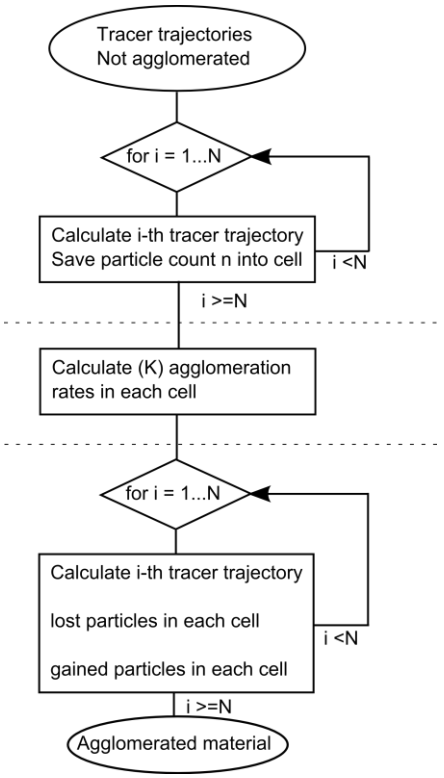

Figure 3: Schematic diagram of the Bus-Stop model.

2.) With this data in each cell the agglomeration rates for each possible pair of particle collisions is calculated. If in a cell a particle with diameter *i* is not present, then the agglomeration rate for all pairs with this class is zero.

3.) The computation of tracer trajectories is repeated and the lost and gained amount of particles can be determined since $K_{i,j}$ were computed in step 2.

Since the smallest particle class can only lose mass, this class is calculated first. The lost particles are stored as (waiting) particles and can be gained by other trajectories. After that all other classes, in diameter increasing order are computed and with lost and gained particles. Finally, particles which are not gained were added to theire particle class. With this restrictive procedure, the mass balance is always fulfilled.

The gain process in detail can be described as follows. If in one cell particles should be gained, then it is checked if free particles of the relevant class are waiting there and then these particles are collected. In detail, the volume (or mass) of the particles is added to the actual class. Hence, this does not change the diameter and also not the way of the trajectory.

De-agglomeration

One problem of the presented agglomeration rates is, that agglomeration only stops after all particles have agglomerated to one big particle. That could not be observed in real systems. Therefore it is reasonable to assume a threshold for the agglomeration rate based on the diameter, for example two particles would agglomerate to a particle with a diameter that is not possible. Hence, this agglomeration must be avoided.

RESULTS

Validation: Agglomeration model

In a first step, the Bus-Stop model was implemented with Lagrangian discretization in MATLAB and FLUENT for a simple 2D case, to compare the results with the discretized Smoluchowski equation using (19). Particles with density of $\rho_p = 2700$ kg/m^3 are freely falling in a pipe of length 50 m and diameter 0.1 m, at their terminal settling velocity. 20 particle classes were used, according to (19) with $d_1 = 5$ µm and the threshold for the agglomeration is set to $d = 92.94$ µm. The particle size distribution is chosen to be Gaussian

$$n_i = C_1 e^{\left(-0.5\left(\frac{d_i - d_C}{d_\sigma}\right)^2\right)}, \qquad (19)$$

with $d_C = 8.75$ µm and $d_\sigma = 1$ µm. With the given volume fraction of the particles ($\alpha_p = 0.3$), C_1 can be easily calculated.

Figure 4, shows the comparison of the particle size distribution at the end of the 50 m pipe between the Bus-Stop model implementations and the Smoluchowski population balance model. It can be seen, that both models, show nearly identical results. The comparison between the Bus-Stop model in MATLAB and FLUENT shows also a small difference. These differences are caused by setting the velocity of particles in the MATLAB model to a fixed value, whereby the particle velocity in FLUENT is computed based on the drag. It is found that the error is approximately 0.1%. However, with this validation, the usage of the Bus-Stop model is justified.

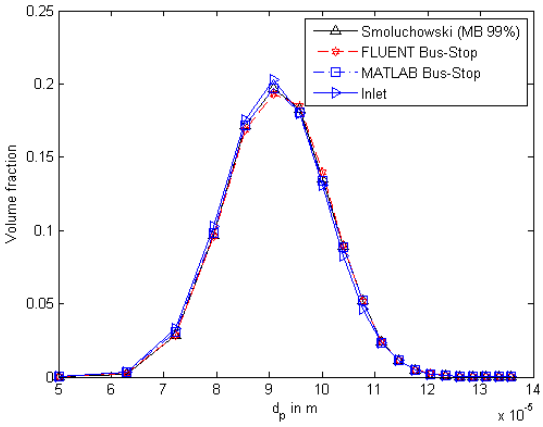

Figure 4: Comparison of particle volume fraction between discretized Smoluchowski model and the Bus-Stop model (in MATLAB and FLUENT)

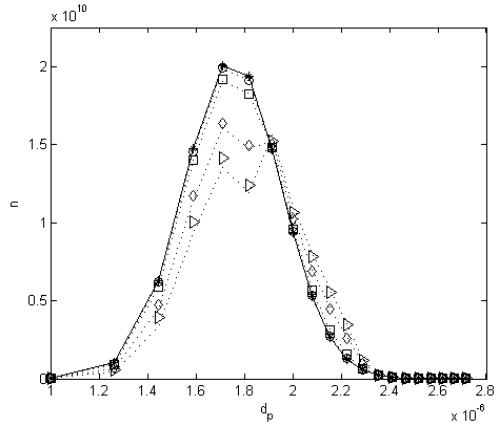

Figure 5: Change of particle size distribution over height (○ 1m, □ 5m, ◇ 25 m and ▷ 50 m) in the vertical pipe. Comparison between Smoluchowski (....) and Bus-Stop model (○,□,◇ and ▷).

Figure 5, shows the change from 1 m to 50 m in the pipe, for a different particle size distribution with $d_1 = 1$ µm, $d_C = 1.75$ µm and $d_\sigma = 0.2$ µm. The Smoluchowski model simulation was stopped after 99% of mass reaches the end of the pipe. Therefore a small error in the mass conservation is present. Nevertheless, this results show on one hand that the Bus-Stop model can be used for the simulation of agglomeration with Lagrangian tracer trajectories and on the other hand, that the Bus-Stop model is provides the same results as the approved Smoluchowski model, hence it can be used for the simulation of centrifugal dust separators.

Application: Cyclone

A cyclone is used to test the agglomeration model at industrial scale application. Geometry and results for the cyclone without modelling agglomeration can be found in Schellander et. al (2012a,b). For the simulation the same

particle size distribution as mentioned before (eq. 19 and Figure 4) was used.

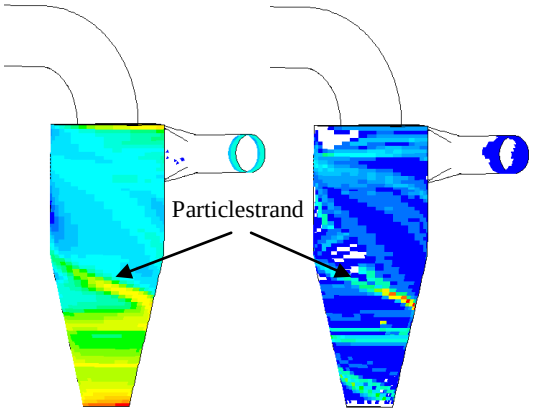

Figure 6: Volume fraction of granular material in the cyclone. On the left side, the Eulerian-Eulerian granular phase and on the right side the coupled Lagrangian tracer trajectories can be seen.

Figure 6 show the volume fraction in the granular phase and the particle amount in the Lagrangian trajectories. In both representations the same particle strand can be seen, this is one result of the coupling between Eulerian granular phase and the tracer trajectories in the EUgran+Poly model.

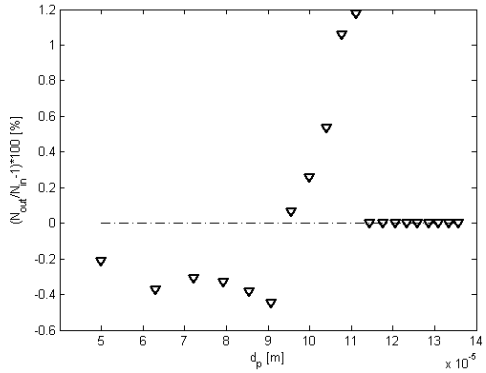

Figure 7: Difference of particle size distribution at the inlet and the particle outlet of the cyclone.

The particle size distribution change by agglomeration was very small, which can be seen in Figure 7. Nevertheless, the movement of smaller particles to bigger ones, by agglomeration is observed. The agglomeration model, increases the separation of the small particles, which is in standard simulation models often not the case. Figure 8 shows the separation efficiency of the cyclone for different models with respect to the particle diameter. The impact on the separation of small particles in the hybrid model EUgran+Poly depends on the model of the poly-dispersed drag law, particle-particle collision model (Schellander et al. 2012b) and the agglomeration model. The agglomeration model increases the separation efficiency in the simulation by 1-4%.

CONCLUSION

The agglomeration model shows how the particle mean diameter increases in the cyclone. This provides a more precisely simulation of the separation efficiency, especially for small particles. The EUgran+Poly model in combination with the Bus-Stop agglomeration model, allows the simulation of granular transport and separation in an more accurate way than the volume balance model.

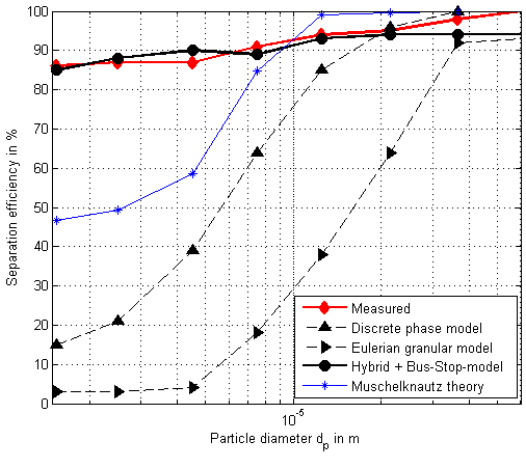

Figure 8: Simulation results of separation efficiency of a cyclone separating limestone granular. The results are compared to measurements and the theoretical curve computed with Muschelknautz theory.

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