The collision efficiency in a shear flow

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Abstract

Fluid flows with cohesive particles are present in oil industry (e.g. natural gas/oil with hydrates, wax or asphaltenes), medicine (e.g. blood cells), nano- and ferro-fluidic applications (e.g. fluids with nanoparticles subject to the van der Waals and electrostatic interactions) and even in astrophysics (e.g. grains in planetary rings). Such flows may lead to formation of agglomerates that, for example in pipelines, may result in unwanted phenomena such as formation of deposits. The main process parameter governing this is the ‘collision efficiency’, which is the ratio of the number of collisions resulting in agglomeration to the total number of collisions. This is commonly considered to depend on the relative magnitudes of attractive and repulsive interactions during a collision. The effect of the particles’ mechanical properties on the agglomeration efficiency has, however, not yet been studied. In this paper the agglomeration efficiency is studied as a function of interparticle friction, stiffness, density and volume fraction by numerical simulation. By running direct numerical simulations (DNS) with Lagrangian particle tracking of a shear flow laden with solid particles, the parameters influencing the agglomeration efficiency are demonstrated.

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and their effects quantified. Finally, an expression that relates the collision efficiency to the salient dimensionless physical parameters is proposed.
1 Introduction

The process of particle agglomeration in flows involving dispersed phases takes place in daily life, in space and in many branches of industry. Blood cells clotting (Gailani and Broze, 1991), wet sand clustering (Kudrolli, 2008), cloud formation (Lehtinen, 1997) and many others are typical examples of processes depending on agglomeration. Less ordinary applications include, for example, nano- (Timofeeva et al., 2007) and ferro-fluidic (Chantrell et al., 1982) clustering and the formation and stability of agglomerates in Saturn’s rings (Albers and Spahn, 2006).

Along with all the positive aspects of the agglomeration process there are numerous drawbacks, mainly linked to channel flows laden with cohesive particulate phases. For example, in the oil industry the agglomeration of asphaltenes (Eskin et al., 2011) or gas hydrates (Balakin, 2010) can block pipelines with an obstructing deposit. Even more dramatically, the vascular stenosis (Feng et al., 2011) is also a consequence of the cohesive agglomeration. For such processes, also in terms of risk management, it is important to estimate the probability of obstruction formation due to agglomeration, which, in turn, is closely related to the particle collision efficiency.

The phenomenon of agglomeration is driven both by the flow or diffusion-induced collisions of particles and the cohesive interaction, which may be caused by different types of forces: electrostatic, van der Waals, liquid bridg-
ing, magnetic etc. The mechanical properties of the particles (density, stiffness, friction coefficient etc.) are also important for the process of inter-particle collision and the probability of a collision leading to agglomeration.

Experimental determination of collision efficiency is a challenging problem which is still not fully solved. Hounslow et al. (2001) proposed a micro-mechanical model for the efficiency of aggregation during the precipitation of inorganic salts from an aqueous solution. They suggested that the efficiency was proportional to the dimensionless ratio in between the mechanical strength of the agglomerating bridge and the flow shear force. The model was validated with experimental data on calcium carbonate and calcium oxalate precipitation in agitated systems. The validation of the model was done using generalized data for the temporal evolution of the particle size distribution moments, since the agglomeration efficiency was not determined empirically. Similar indirect estimates of collision efficiency on the basis of experimental information on the temporal variation of particle size distributions were made in e.g. Oles (1992) and Heath et al. (2005).

Agarwal (2002) studied the process of the shear-induced flocculation of polymer particles with the use of in-situ microscopy. The work was focused on determining the collision efficiency on basis of the temporal variation in the number concentration of particles. Like in Hounslow et al. (2001), the calculation of collision efficiency implied the use of an assumed expression for the frequency of inter-particle collisions.

Theoretical studies of agglomeration shed light on the details of the process. For example, in the paper by van de Ven and Mason (1977) the formation of two-particle agglomerate is considered on the basis of trajectory analysis.
The collision efficiency is found to depend on the ratio between van der Waals force and the drag force. The collisions are, however, not modelled directly so that the effects of some relevant parameters, such as friction and plastic deformation during the collision, are not accounted for.

Although many numerical models studying agglomeration have been produced recently (e.g. Brilliantov et al. (2007); Hollander et al. (2001); Freireich et al. (2009)) only a few study the collision efficiency. The work by Ho and Sommerfeld (2002) is a rare exception as, among other interesting issues, the paper considers the agglomeration efficiency as a function of the volume fraction, size distribution and the Stokes number of the particles.

In this present article the process of agglomeration of cohesive particles in a shear flow is studied. This was done with the use of an in-house numerical code that enables the multi-parametrical study of the collision efficiency. Special attention is paid to the influence of the mechanical properties of the particles on the collision efficiency. An expression relating the collision efficiency to a set of dimensionless parameters incorporating the relevant physical parameters is given (Eq. 18).

2 Model description

Although the current model includes some specific features described below, its main principle is based on the standard Lagrangian technique for the multiphase flow simulation, explained in, for example, Crowe et al. (1998). Thus the dispersed phase is modelled using the single-particle equations of motion
for linear momentum and torque:

\[ m_i \frac{d\vec{V}_i}{dt} = \vec{F}_i, \]  

(1)

where \( \vec{V}_i \) is the velocity of \( i^{th} \) particle and \( m_i \) is its mass. In the current model \( \vec{F}_i \) is just the drag force, calculated as:

\[ \vec{F}_i = \frac{\pi}{8} d_i^3 C_{D,i} \rho_f (\vec{U} - \vec{V}_i) \left| \vec{U} - \vec{V}_i \right|, \]  

(2)

where \( d_i \) is the diameter of \( i^{th} \) particle, \( C_{D,i} \) is its drag coefficient, \( \rho_f \) is density of the carrier phase and \( \vec{U} \) is the velocity of the carrier phase. For the torque:

\[ I_i \frac{d\vec{\omega}_i}{dt} = \vec{M}_i, \]  

(3)

where \( I_i \) is the particle moment of inertia, \( \vec{\omega}_i \) is the particle angular velocity and \( \vec{M}_i \) is the torque acting from the fluid, which is actually assumed to be negligibly low for the cases simulated in this paper. The particle angular velocity can thus change only due to collisions with other particles or walls.

The force and the moment acting during collisions are not included in Equations (1) and (3), since a hard-sphere model is used for the collisions.

The flow of the carrier phase, liquid in this case, is described by the Navier-Stokes equations:

\[ \nabla \vec{U} = 0, \]  

(4)

\[ \rho_f \frac{D\vec{U}}{Dt} = -\nabla p + \mu \nabla^2 \vec{U} + \vec{F}, \]  

(5)

where \( p \) is the pressure, \( \mu \) is the dynamic viscosity of the carrier phase and \( \vec{F} \) is the net drag force acting on the \( n_p \) particles per unit volume of suspension:
\[ \vec{F} = \sum_{i=1}^{n_p} \vec{F}_i. \]

Equations (1–5) constitute a self-contained model that describes an incompressible flow with solid particles. This was also used in a previous paper by some of the present authors (Kosinski et al., 2009), where the computational code was validated against benchmarks and experimental observations. Interactions between the particles were, however, neglected in that work.

One of the objectives of this paper is to investigate inter-particle collisions, and for this purpose the hard-sphere model, extended to take into account ad- and cohesion, was used. This was described in Kosinski and Hoffmann (2010) and is based on the standard hard-sphere model described in Crowe et al. (1998), probably first published by Matsumoto and Saito (1970). This model was also discussed in previous papers by some of the present authors (Kosinski and Hoffmann, 2010; Ilea et al., 2008).

The standard (i.e. without cohesion between the particles) model is based on writing equations for the impulse acting on the colliding particles formulated with use of two additional parameters: the restitution coefficient, accounting for the loss of mechanical energy due to plastic deformation, and the Coulombian friction coefficient accounting for the particle surfaces sliding over each other during the collision. This system of equations relates the post-collisional velocities to the pre-collisional ones as illustrated in Fig. 1. Details are given in Kosinski et al. (2005); Kosinski and Hoffmann (2005, 2007).

The standard hard-sphere approach cannot be used to study agglomeration because it does not take into account cohesive/adhesive interactions.
Fig. 1. The concept of the extended hard-sphere model shown for a two-dimensional collision, where two (non rotating) particles approach each other with velocities \( v_1^{(0)} \) and \( v_2^{(0)} \) and, if they do not agglomerate, leave the collision with velocities \( v_1 \) and \( v_2 \) and angular velocities \( \omega_1 \) and \( \omega_2 \), while, if agglomerating, the agglomerate leaves with velocity \( v \) and angular velocity \( \omega \).

The concept of the extended (Kosinski and Hoffmann, 2010, 2009) model is sketched in Figure 1 in a 2-D representation. Two particles approach a collision with the velocities \( v_1^{(0)} \) and \( v_2^{(0)} \). The impulses acting on particle 1 are shown in the figure, where \( J_{n,a} \) and \( J_t \) are the normal and tangential components of the impulse according to the classical hard-sphere model. \( J_{n,c} \) is the additional impulse acting due to cohesive interaction, assumed to act normal to the plane of impact.

The existence of \( J_{n,c} \) means that the colliding particles enter a potential well, from which they may or may not escape depending on the mechanical energy lost during the collision due to dissipative processes, such as any plastic deformation of the particles during the impact. The agglomeration criteria are obtained by comparing the momentum of the particles as they just leave the
collision with that necessary to escape the potential well. The final criteria are
given in the Figure 1, and with expressions for the impulse acting during the
collision according to the classical hard-sphere model:

$$J_{n,a} = -m(1 + e)(\vec{n} \cdot \vec{G}_0),$$

(6)

where $\vec{G}_0 = \vec{v}_1(0) - \vec{v}_2(0)$, $\vec{n}$ is the unit vector normal to the plane of collision,
$m = \frac{m_1 m_2}{m_1 + m_2}$ is the effective mass of the colliding particles and $e$ is the coefficient
of restitution.

And for the limiting normal and tangential impulses leading to agglomeration:
$J_{nl} = -m(\vec{n} \cdot \vec{G}_0)$ and $J_{tl} = -m(\vec{t} \cdot \vec{G}_0)$, $t$ - tangential unit vector, these criteria
become:

$$J_{n,c} > m e(\vec{n} \cdot \vec{G}_0) \quad \text{and} \quad J_t > -m(\vec{t} \cdot \vec{G}_0)$$

(7)

The expression for $J_{tl}$ given above and the second agglomeration criterion
in Figure 1 has given us the opportunity to correct the two typing errors
in Kosinski and Hoffmann (2010), which were in Equations (18) and (21) in
that paper. Only the first of the two criteria in Eq. (7) applies in case of
collisions where the particles stop sliding over each other during the collision.

These criteria can be rewritten into a criterion for the resultant of the pre-
collisional particle relative velocity, which, for agglomeration to take place,
must be below a limiting value, $G_{0}^{cr}$:

$$G_{0}^{cr} = \left(\frac{a}{\epsilon m}\right)^{\frac{5}{6}} \sqrt{1 + f^2(1 + 2e)^2}$$

(8)
where $f$ is the friction coefficient and $a = J_{n,c}(\vec{G}_0 \cdot \vec{n})^{0.2}$. The first of these criteria applies in cases where the particles slide throughout the collision, the second in cases where the particles stop sliding during the collision (Crowe et al., 1998; Kosinski and Hoffmann, 2010).

The value of the cohesive impulse was estimated in Kosinski and Hoffmann (2010) by integration of the expression for cohesive van-der-Vaals force (Israelachvili, 1992) over the duration of impact of two elastic bodies (Stronge, 2000; Tsuji et al., 1992). This corresponded to e.g. dry, spherical, beads.

The model for the cohesive impulse was:

$$J_{n,c} = 0.238 \left( \frac{m^2}{E_\ast^2 (G_0 \cdot \vec{n})} \right)^{\frac{1}{5}} \frac{A r^{\frac{4}{5}}}{D_c^2},$$

where:

- $r$ is the effective particle radius: $\frac{r_1 r_2}{r_1 + r_2}$,
- $E_\ast$ is the effective Young’s modulus defined as: $\frac{E}{2(1-\sigma^2)}$ with $\sigma$ and $E$ being the particle Poisson coefficients and their Young’s moduli,
- $A$ is the Hamaker constant
- $D_c$ is the separation distance during contact (usually assumed to be equal to 0.2 nm (Israelachvili, 1992)), and

Work is in progress to quantify the cohesive impulse more accurately and this will be published in a separate paper.

In the current model it is assumed that the fractal structure of the agglomerate formed does not significantly influence its further mechanics. Keeping this assumption in mind, the agglomerate size is calculated on the equivalent
In order to study the agglomeration of particles in a shear flow the geometrical and boundary conditions of the process are configured so that two goals can be fulfilled: obtaining an approximately linear velocity profile (Couette flow) of the carrier phase and achieving a sufficiently long process duration. A rectangular domain (see Fig. 2) of size 39 × 39 mm, meshed by 64 × 64 × 1 finite volume cells was used in the model. A symmetry boundary condition was applied to both front and back planes of the domain, reducing Eqs. (4) and (5) to a two-dimensional formulation, which, in turn, reduces Eq. (10) to an area-conservation principle: \[ d_{agg} = \sqrt{d_1^2 + d_2^2}. \]

The desired velocity profile is established with the use of oppositely directed moving walls (boundary conditions for Eqs. (4) and (5)), located on the horizontal sides of the domain. The interactions of the dispersed phase with the walls were set according to the standard hard-sphere model (Crowe et al., 1998; Ilea et al., 2008) with a restitution coefficient equal to 1.0 and a friction coefficient of 0.15. The vertical sides of domain were equipped with periodic boundary conditions making it possible to prolong the duration of the process by continuous ‘recirculation’ of both phases.

The initial conditions for Eqs. (1–5) were: \( \vec{U} = 0, \vec{V}_i = 0, p = p_b, d_i = d_0 \), where \( p_b \) is the reference pressure and \( d_0 \) is the size of initial, primary particle.

The equations were solved with the modified Chorin-Temam technique (Griebel et al., 1997), where the convective terms were discretized using the variable-order nonoscillatory scheme (Varonos and Bergeles, 1998) and solved tempo-
Fig. 2. Schematic representation of the numerical domain and the boundary conditions.

rally by the Euler explicit scheme (more details are available in Kosinski et al. (2009)). In addition, in order to account for drag interaction as accurately as possible, the fluid velocity values were linearly interpolated between grid points when evaluating the drag-force necessary for Eq. (1). The time-step was calculated according to the standard Courant-Friedrichs-Levy condition. The physical properties of both phases and other parameters of the process are presented in Table 1.

3 Results and discussion

The particle collision efficiency was determined as the ratio of the number of collisions leading to agglomerate formation, $N_{agg}$, to the total total number of
Table 1

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Shear rate, $\gamma$</td>
<td>71 s$^{-1}$</td>
</tr>
<tr>
<td>Restitution coefficient, $e$</td>
<td>0.9</td>
</tr>
<tr>
<td>Primary particle size, $d_0$</td>
<td>25.0 $\mu$m</td>
</tr>
<tr>
<td>Friction coefficient, $f$</td>
<td>0.15</td>
</tr>
<tr>
<td>Fluid dynamic viscosity, $\mu$</td>
<td>0.001 Pas</td>
</tr>
<tr>
<td>Separation distance, $D_c$</td>
<td>0.2 nm</td>
</tr>
<tr>
<td>Fluid density, $\rho_f$</td>
<td>1000 kg/m$^3$</td>
</tr>
<tr>
<td>Particle area fraction, $\phi$</td>
<td>6.5$\cdot$10$^{-3}$</td>
</tr>
<tr>
<td>Hamaker constant, $A$</td>
<td>1.6$\cdot$10$^{-21}$ J</td>
</tr>
<tr>
<td>Poisson ratio, $\sigma$</td>
<td>0.3</td>
</tr>
<tr>
<td>Youngs modulus, $E$</td>
<td>3.3$\cdot$10$^{10}$ Pa</td>
</tr>
<tr>
<td>Cavity size</td>
<td>39 mm</td>
</tr>
</tbody>
</table>

Collisions, $N_{tot}$, (please note that these parameters are time-dependent):

$$\alpha = \frac{N_{agg}}{N_{tot}}$$  \hspace{1cm} (11)

In other words, the parameter, defined by Eq. (11), represents the statistical probability of a collision leading to agglomeration. From the description of the model, presented in the previous section, it follows that $\alpha$ can be considered to be a function of a set physical variables, which govern the process of agglomeration:

$$\alpha = f(\gamma, d_0, D_c, \mu, \rho_d, A, E^*, f, e, \phi)$$  \hspace{1cm} (12)

Applying the Buckingham II-theorem (Buckingham, 1914), the efficiency can be considered to depend on the following dimensionless groups:

$$\alpha = f(I_1, I_2, I_3, I_4, f, e, \phi)$$  \hspace{1cm} (13)

where:
\[ I_1 = \frac{(6\pi \mu \gamma d_0^3)}{(8\mu A)} \] is the ratio between the attractive van-der-Vaals interaction and repulsive flow force, also known as the flow number $Fl$

\[ I_2 = \frac{(\gamma \rho_d d_0^2)}{(18\mu)} \] is the measure of particles inertia also known as the Stokes number $St$

\[ I_3 = \frac{D_c}{d_0} \] relates the efficiency of agglomeration to the minimum possible separation between the particles

\[ I_4 = \frac{E^*}{(\mu \gamma)} \] represents the ratio between stiffness of the particles and the flow force

3.1 Parameter effects on collision efficiency

As mentioned in the previous section, the simulations started from zero velocity field, and therefore with no interactions between the particles. As the boundaries started to move, a sharp agglomeration efficiency increase was observed during the first 4 seconds of the process (Fig. 3), which corresponds to approximately 300 characteristic times of the system (defined as the reciprocal of the shear rate). During this initial period, before the fluid velocity field is established, there will be a very high local shear rate at the walls, where also any particle collisions will take place, and low shear in the middle of the domain. It therefore stands to reason that the collision efficiency should start at a low value and increase as the steady-state fluid velocity field is established.

Later in the process the agglomeration efficiency can be seen to decrease slowly. This is caused by an increase in the particle size with time due to coagulation (Eq. (10)). Equation (8) shows that, all else being constant, including the particle relative velocity, the collision efficiency will decrease with increasing particle size.
The process involves decrease of the total number of particles in the system due to agglomeration, and it can therefore be associated with the zeroth moment of the particle size distribution (PSD) (Balakin et al., 2011, 2010):

\[ M_0 = \int g(r)dr, \quad (14) \]

which represents the total number of particles with the number-density size distribution \( g(r) \) in unit volume of suspension. It is known from the population balance approach (Hounslow et al., 1988; Hounslow, 1990) that the rate of change of the zeroth PSD moment may be related to the rate of particle agglomeration through an expression of type:

\[ \frac{dM_0}{dt} = -0.5\alpha Km_0^2, \quad (15) \]

where \( K \) represents the probability that a given particle pair will collide within a second and \( 0.5M_0^2 \) is the number of distinct particle pairs in 1 m\(^3\) of suspension. For particles with sizes below the Kolmogorov length scale, the

Fig. 3. Collision efficiency as a function of time during start-up. Model parameters are as given in Table 1.
steady-state collisional frequency can be expressed with a relation developed by Saffman and Turner (1956):

\[ K = 0.31 \gamma \left( v_i + v_j \right)^3, \]  

(16)

where \( v_i \) and \( v_j \) are the volumes of the particles and \( \gamma \) is the shear rate.

Integration of Eq. (15) gives an expression for \( M_0 \) as a function of time:

\[ M_0(t) = \frac{M_0(0)}{1 + 0.5\alpha K M_0(0)t}. \]  

(17)

Substituting the collision rate from Eq. (16) into Eq. (17) it is possible to compare the variation in \( M_0 \) predicted theoretically by Eq. (17), with the variation in the simulations described in the previous section. The comparison is shown in Fig. 4 where the moment is scaled by its initial value for different values of a time. The collision efficiency, \( \alpha \), used in Eq. (17) was taken from the simulation results. It can be seen in Fig. 4 that the time-variation in the PSD moment from the simulations is comparable to the theoretical one. The rate of collisions leading to agglomeration is, however, approximately twice higher in the simulations than predicted by theory during the first seconds.

This observation is actually consistent with the results presented in some other papers (Chen et al., 1998; Sundaram and Collins, 1997; Zaichik et al., 2006) where the theoretical frequency by Saffman and Turner (1956) was also found to be overestimated. The simulation results converge to the theoretical predictions at higher simulation times.

The process of agglomeration, which is reproduced by the simulations, is illustrated in Fig. 5 in terms of the number-average particle size as a function of time and the PSDs at two points in time: 5 and 50 s. The mean particle
Fig. 4. Temporal evolution of $M_0$. The theory, represented by Eq. (17) is compared with simulation results. The model parameters are given in Table 1.

size in the top figure is scaled by its initial value $d_0$, shown in Table 1.

During the first 40 seconds of the process, the particle size increases almost linearly with a factor of about four, whereafter the system begins to stabilize due to the decrease in the number of particles and the collision efficiency. The bottom part of the figure shows the dramatic change in the number size distribution of the particles.

The results of the simulations were further compared with theoretical investigations done by other researchers who related the collision efficiency to the flow number, $Fl$, which was derived above using dimensional analysis (Eq. (13), group $I_1$). In Fig. 6 the collision efficiency obtained in the simulations is compared to an expression proposed for the collision efficiency of two primary particles by van de Ven and Mason (1977), namely $\alpha \approx Fl^{-0.18}$. It can be seen in the figure that the probability of particles agglomeration is inversely related to the magnitude of the flow number and this is in agreement with Ven and Mason. However, the simulation results show a much stronger dependence than Ven and Mason’s analytical relation. A possible reason is that our model
Fig. 5. (A) The number average particle size as a function of time. (B) PSDs for 5 and 50 s simulation time. Model parameters are given in Table 1

does not account for inter-particle viscous retardation (Adams and Edmondson, 1987). This effect constitutes an additional dissipative loss of mechanical energy for the colliding particles, and will therefore lead to decreased collision efficiency.

A comparison of the present simulation results with the later theoretical relation proposed by Bäbler (2008) for the estimation of collision efficiency for polysized fractals (Figure 5 in the original paper of Bäbler) gives better agree-
ment. The model results can be seen to predict a slightly lower collision efficiency. This may be explained by the use of the equivalent diameter approach for estimating the size of the agglomerates instead of estimating the size assuming a fractal structure.

![Graph](image.jpg)

**Fig. 6.** Temporary-average collision efficiency as a function of system flow number $F_l = 6\pi \mu \gamma d^3/(8A)$. Model parameters are given in Table 1.

It was further shown by Ho and Sommerfeld (2002) that the agglomeration efficiency is inversely related to the magnitude of the particle Stokes number meaning that a longer response time of the particles decreases the probability of agglomerate formation. The Stokes number is proportional to the square of the particle diameter, and, as discussed above, the agglomeration model used in this present work predicts that the collision efficiency decreases with increasing particle diameter. In the present simulations, therefore, a similar dependence on the Stokes number is observed, as shown in Figure 7.

The area fraction of the dispersed phase is the dimensionless parameter representing the concentration of particles in the system. Figure 8 shows that the particle concentration has only a minor influence on the collision efficiency (note the expanded scale of the ordinate in the figure). A slight reduction in
the collision efficiency is, however, observed with an increase in the particle concentration. Again, this observation is consistent with the results of Ho and Sommerfeld (2002). A possible explanation for this may be that an increase in the particle concentration will cause the mean particle size to increase faster, and larger particles have, as noted above, a lower critical aggregation velocity.

Equation (9) shows that an increase in separation distance causes reduction in the adhesive impulse $J_{n,c}$. According to Eq. (8); the critical value of relative
velocity then also decreases, reducing the collision efficiency. In order to test
the sensitivity of the results to this parameter a series of simulations were
carried out, the result of which are shown in Fig. 9. The variation seen in the
figure confirms the validity of the numerical scheme applied.

![Fig. 9. Temporary-average collision efficiency as a function of dimensionless surface separation at contact, $D_c/d$. Model parameters are given in Table 1.](image)

3.2 The effects of the particle mechanical properties

Both inelastic particle deformation and friction during collisions will rob the
particle phase of mechanical energy, which is, in turn, likely to lower the
average relative velocities of colliding particles. A lower relative velocity will, as
mentioned, increase the collision efficiency. The friction coefficient also appears
directly in one of the expressions for $G_0^{cr}$ in Eq. (8), such that increasing $f$
leads to an increase in $G_0^{cr}$, increasing the collision efficiency. The effect of $f$
on the collision efficiency is shown in Fig. 10. It can be seen that $f$ does not
have a very strong influence on $\alpha$.

The particle stiffness, represented by the effective Young modulus, is present
in the dimensionless group $I_4$. Figure 11 shows clearly that “softer” particles
Fig. 10. Temporary-average collision efficiency as a function of friction coefficient $f$. Model parameters are given in Table 1.

agglomerate more, which can be explained by the longer duration of contact during collision.

Fig. 11. Temporary-average collision efficiency as a function of $I_4 = E^*/\mu \gamma$. Model parameters are given in Table 1.

As mentioned, the other parameter, in addition to $f$, determining the loss of mechanical energy during collisions is the inelastic part of the particle deformation, described by the coefficient of restitution, $e$. More importantly $e$ also appears directly in the agglomeration criterion, Eq. (8), showing that an increase in $e$ will decrease $G^*_0$, and therefore increase the collision efficiency,
In Fig. 12 collision efficiency is presented as a function of the restitution coefficient $e$ and the qualitative variation in $\alpha$ is consistent with what one would expect from the analytical relation.

![Graph](image.png)

Fig. 12. Temporary-average collision efficiency a function of restitution coefficient $e$.

### 3.3 Model limitations and summarized expression for the collision efficiency

The cohesive interaction has been assumed to be van der Waals forces. Liquid bridging (Israelachvili, 1992) may, in many practical cases, give rise to a much stronger cohesive force, for example in granulation (Chua et al., 2011) or for water-wet particles dispersed in oil. Thus the presence of liquid films on the particles would increase the collision efficiency. The elastic coefficient of restitution (neglecting the cohesion, see Kosinski and Hoffmann, 2010), $e$, is assumed constant and determined only by the material properties of the particles. According to, e.g. Brilliantov et al. (2007), this parameter may well vary with the pre-collisional velocity.

Once formed, and after finding the post-collisional velocities, the agglomerates are taken as volume-equivalent spheres. However, a fractal agglomerate
behaves differently during a collision and is subject to a different fluid-solid interaction. Kusters et al. (1997) finds that the collision efficiency increases with a decrease in fractal dimensionality. Also, porous flocs agglomerate approximately 3 times more efficiently than solid spheres at the same fractal dimension. Shear-induced breakage of particles which takes place in the real systems (Spicer and Pratsinis, 1996) is not accounted for by the model.

The simulations carried out were in the turbulent flow regime at Reynolds numbers around 27000. The mesh size was 5–11 Kolmogorov length scales, so that the simulations are not fully DNS. There were no turbulent eddies formed during the simulations, and it can be claimed that the results for collision efficiency are valid for simple shear flow, such as would be encountered within a single turbulent eddy. In addition, the spectrum of two-dimensional turbulence is different from real 3D. Three-dimensional agglomeration would also change the geography of interparticle collisions. For example, in the work by Liu and Schwarz (2009) it is shown that the agglomeration efficiency predicted in 3D simulation is 1.5–2.0 times larger than the efficiency predicted for 2D.

Based on all the effects described in this paper it is possible to construct a relation $\alpha = f(Fl, St, D_c/d_0, I_4, f, \phi, e)$ by fitting it to the results of the simulations. This was done with the use of the multidimensional Rosenbrock search technique (Conn et al., 1988). The results of the optimisation are presented in Fig. 13 where the agglomeration efficiency is found to be approximated with the expression:

$$\alpha = 0.19Fl^{-0.48}St^{-0.13} \left( \frac{D_c}{d_0} \right)^{-1.11} I_4^{-0.26} f^{0.27} \phi^{-0.01} e^{-1.06}$$  \hspace{1cm} (18)

Pearsons $r$ for the data fitted by eq. (18) is 0.96.
Expression 13 is valid for the following parameter intervals: $Fl \in (1 \cdot 10^5, 24 \cdot 10^5)$, $St \in (0.2 \cdot 10^{-3}, 2.6 \cdot 10^{-3})$, $\frac{D_c}{d_0} \in (4 \cdot 10^{-6}, 24 \cdot 10^{-6})$, $I_4 \in (7 \cdot 10^9, 930 \cdot 10^9)$, $f \in (0.15, 0.50)$, $\phi \in (2 \cdot 10^{-3}, 7 \cdot 10^{-3})$, $e \in (0.3, 1.0)$ and $Re \in (10000, 40000)$.

4 Concluding remarks

A numerical study of the collision efficiency for cohesive particles in a shear flow has been performed using a Eulerian-Lagrangian in-house code, validated in multiple case studies together with a hard-sphere collision model extended to take into account cohesion between the colliding particles.

A dimensional analysis of the process formulated seven dimensionless groups, which affected the collision efficiency: flow number, Stokes number, dimensionless separation distance, dimensionless stiffness of the particles, friction coefficient, area fraction of particles and the coefficient of restitution.
The variation of the collision efficiency with all these variables were studied by simulation and the results are presented in the paper.

After an initial start-up effect, $\alpha$ was found to decrease slowly in time, partly due to an increase in the particle size as agglomeration proceeded.

It was found that the rate of agglomeration was comparable to the rate predicted by a relation due to Saffman and Turner. However, it was observed that the collision efficiency in the simulations was somewhat higher than that predicted, something that has also been found in other numerical studies.

Also the relations of Bäbler and Ven and Mason predict collision efficiencies of the same order as those obtained in the simulations.

An approximate expression relating the agglomeration efficiency to the dimensionless parameters was generated.

**Nomenclature**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A$</td>
<td>Hamaker constant</td>
<td>(J)</td>
</tr>
<tr>
<td>$a$</td>
<td>intermediate parameter from Eq.8</td>
<td>(kg·m$^{1.2}$/s$^{1.2}$)</td>
</tr>
<tr>
<td>$C_D$</td>
<td>drag coefficient</td>
<td></td>
</tr>
<tr>
<td>$D_c$</td>
<td>separation distance during contact</td>
<td>(m)</td>
</tr>
<tr>
<td>$d$</td>
<td>diameter of particle</td>
<td>(m)</td>
</tr>
<tr>
<td>$E$</td>
<td>Young’s modulus</td>
<td>(Pa)</td>
</tr>
<tr>
<td>$E_*$</td>
<td>effective Young’s modulus</td>
<td>(Pa)</td>
</tr>
<tr>
<td>$e$</td>
<td>coefficient of restitution</td>
<td></td>
</tr>
<tr>
<td>$F$</td>
<td>drag force</td>
<td>(N)</td>
</tr>
</tbody>
</table>
$Fl$ flow number

$f$ coefficient of friction

$G_0$ pre-collisional relative velocity ($m/s$)

$g(r)$ particle size distribution function ($m^{-4}$)

$I$ dimensionless criteria

$J$ moment of inertia ($kg\cdot m^2$)

$J_{n,a}$ normal component of the impulse ($kg\cdot m/s$)

$J_{n,c}$ cohesive impulse ($kg\cdot m/s$)

$J_t$ tangential component of the impulse ($kg\cdot m/s$)

$J_{nt}, J_{dt}$ normal and tangential limiting impulses ($kg\cdot m/s$)

$K$ rate of collisions ($m^3/s$)

$M$ torque ($N\cdot m$)

$M_0$ 0$^{th}$ moment of particle size distribution ($m^{-3}$)

$m$ effective mass of colliding particles (kg)

$m_i$ mass of $i^{th}$ particle (kg)

$N$ amount of particles within the system

$n$ unit vector normal to the plane of interparticle collision

$n_p$ amount of particles within the computational cell

$p$ pressure (Pa)

$Re$ Reynolds number

$r$ effective radius of particle (m)

$St$ Stokes number

$t$ tangential unit vector

$t$ time (s)

$U$ velocity of the carrier phase ($m/s$)

$V$ velocity of particle ($m/s$)
\( v^{(0)} \)  
pre-collisional velocity of particle  
(m/s)

\( v \)  
volume of particle  
(m³)

**Greek letters**

\( \alpha \)  
collision efficiency

\( \phi \)  
particle area fraction

\( \gamma \)  
shear rate  
(1/s)

\( \mu \)  
fluid dynamic viscosity  
(Pas)

\( \omega \)  
angular velocity of particle  
(1/s)

\( \rho \)  
density  
(kg/m³)

\( \sigma \)  
Poisson ratio

**Subscripts, superscripts**

\( agg \)  
agglomerate

\( b \)  
reference

\( cr \)  
critical

\( D \)  
drag

\( D \)  
fluid

\( i \)  
number of particle

\( tot \)  
total

\( 1, 2 \)  
particle number in case of their collision

\( 0 \)  
initial condition

28
References


Matsumoto, S., Saito, S., 1970. Monte Carlo simulation of horizontal pneumatic conveying based on the rough wall model. Journal of Chemical Engi-


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