Modelling of coagulation efficiencies in rotating systems

M. Breitling & M. Piesche
Institute of Mechanical Process Engineering,
University of Stuttgart, Germany

Abstract

Under the influence of an induced shear and centrifugal field, inter-particle collisions of solid particles in liquids as well as viscous forces result in agglomeration, breakage, and erosion. There is a permanent alteration of the particle size distribution which is described mathematically by the method of population balances. Due to the uniform surface charge of the dispersed particles, a self-induced agglomeration does not take place automatically which means that coagulant agents need to be added to the suspension. The influence of these electrolytes is taken into account by the so-called coagulation efficiency. In the course of this work, two different models are developed describing the collision efficiency locally and in dependence on apparatus geometry, operating conditions, particle combination (species and mass), coagulant agents and material properties. It is shown that in highly rotating systems particle collisions result in small agglomerates although being exposed to large centrifugal forces and shear forces.

Keywords: coagulation efficiency, populations balances, centrifuge, suspension, multiphase flow.

1 Introduction

In mechanical separation units rotating apparatuses are relatively common. Especially highly rotating disc stack centrifuges become increasingly popular due to their good separation efficiency and the disbandment of filter media. Since the separation is exclusively caused by different densities of the phases, disc stack centrifuges are adapted for the separation of all kinds of dispersed systems (emulsions, aerosols, and suspensions). By using coagulating agents which induce the formation of agglomerates, the separation of very small particles becomes more efficient.
With regard to the flow field in a single gap of a disc stack centrifuge, fig. 1 and table 1, inter-particle collisions of solid particles in liquids as well as viscous forces result in agglomeration, breakage and erosion. There is a permanent

Figure 1: Sketch of a single gap of a disc stack centrifuge.

Table 1: Geometry data.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Angle of the conical gap</td>
<td>$\alpha = 30^\circ$</td>
</tr>
<tr>
<td>Height of the outer annular gap</td>
<td>$h_r = 71$ mm</td>
</tr>
<tr>
<td>Height of the inlet</td>
<td>$h_e = 6$ mm</td>
</tr>
<tr>
<td>Width of the gap</td>
<td>$b = 4$ mm</td>
</tr>
<tr>
<td>Radius of the outer annular gap</td>
<td>$r_a = 100$ mm</td>
</tr>
<tr>
<td>Radius of the inner annular gap</td>
<td>$r_m = 20$ mm</td>
</tr>
<tr>
<td>Radius of the end of the conical gap</td>
<td>$r_i = 30$ mm</td>
</tr>
</tbody>
</table>
alteration of the properties of the dispersed particles, namely the size distribution which cannot be described mathematically by commonly used Euler–Euler or Euler–Lagrangian approaches. In order to take this alteration into consideration, the method of population balances is used. It describes particle numbers \( N \) with certain properties \( \vec{e} = (e_1, e_2, \ldots, e_n) \) in dependence on time \( t \) and position \( \vec{x} = (x_1, x_2, x_3) \). Assuming incremental differences of particle properties and a sufficient large number of dispersed particles, the particle number density function \( f \) is defined by

\[
f(\vec{x}, \vec{e}, t) = \frac{dN}{dx_1 dx_2 dx_3 de_1 de_2 \cdots de_n}.
\]  

For laminar flow patterns, the particle interactions are examined locally in a single gap of a disc stack centrifuge with respect to particle species (non-aggregated particles and agglomerates), particle mass \( m \), and time. The population balance in cylindrical co-ordinates \((x, y, z)\) is then given by

\[
\frac{\partial f(\vec{x}, m, t)}{\partial t} = -\frac{1}{x} \frac{\partial}{\partial x} (xu_l \cdot f) - \frac{1}{x} \frac{\partial}{\partial y} (v_l \cdot f) - \frac{\partial}{\partial z} (w_l \cdot f) + S^+ - S^-
\]  

with velocity components in radial, azimuthal and axial directions \((u_l, v_l, w_l)\). The source term \( S^+ \) describes particle interactions resulting in particles or agglomerates of mass \( m \) by coagulation of smaller particles or by breakage and erosion of larger ones. The sink term \( S^- \) indicates the loss of particles of size \( m \). Except for coagulation efficiencies, their specific inter-particle kinetics have been investigated sufficiently for laminar flows, see Lu and Spielman [1], Schuetz [2], and Smoluchowski [3].

2 Microscopic model

Generally, the coagulation efficiency is defined to be the probability with which a particle collision results in an agglomerate. With respect to the microscopic model, particle trajectories are derived from microhydrodynamic investigations. Since inertia plays a negligible role on the microscale, the hydrodynamic force balances the centrifugal and colloidal forces. The motion of the particles dictates the evolution of the suspension microstructure. The multiparticle configuration in turn shapes the forces \( \vec{F} \) acting on the particles. Solving the mobility problem of two particles, so-called limiting trajectories can be determined defining a capture cross section, see fig. 2. The ratio of the curvilinear particle flux through this section to that of the rectilinear particle flux corresponds to the collision efficiency.

2.1 Particle trajectories

Neglecting torques acting on each particle \( \alpha = 1, 2 \), trajectories can be determined from the mobility problem, Batchelor [4], Kim and Karrila [5]. For cylindrical co-
Figure 2: Sketch of particle trajectories and the capture cross section.

The coupled system of non-linear equations is given by

\[
\frac{dx_α}{dt} = u_\ell - \mu^{-1} \sum_{j=1}^{3} a_{1j}^{(α1)} F_{1j} - \mu^{-1} \sum_{j=1}^{3} a_{1j}^{(α2)} F_{2j} - \sum_{j=1}^{3} \sum_{k=1}^{3} E_{jk} g_{1jk}^{(α)} \tag{3}
\]

\[
\frac{dy_α}{dt} = \frac{1}{x_α} \left[ v_\ell - \mu^{-1} \sum_{j=1}^{3} a_{2j}^{(α1)} F_{1j} - \mu^{-1} \sum_{j=1}^{3} a_{2j}^{(α2)} F_{2j} - \sum_{j=1}^{3} \sum_{k=1}^{3} E_{jk} g_{2jk}^{(α)} \right] \tag{4}
\]

\[
\frac{dz_α}{dt} = w_\ell - \mu^{-1} \sum_{j=1}^{3} a_{3j}^{(α1)} F_{1j} - \mu^{-1} \sum_{j=1}^{3} a_{3j}^{(α2)} F_{2j} - \sum_{j=1}^{3} \sum_{k=1}^{3} E_{jk} g_{3jk}^{(α)} \tag{5}
\]

with \( E \) being the rate of strain tensor, \( a_{ij}^{(αβ)} \) and \( g_{ijk}^{(α)} \) being the scalar mobility functions of the grand mobility matrix (Kim and Karrila [5]) and \( \mu \) being the dynamic viscosity.

### 2.1.1 External forces

In combination with the centrifugal force, the colloidal force

\[
F_{α,\text{colloid}} = -\frac{d}{d|r|} (V_{\text{attr}} + V_{\text{rep}}) \tag{6}
\]

balances the microhydrodynamic force. Applying the DLVO theory (Verwey and Overbeek [6], Derjaguin and Landau [7]), the total potential energy of interaction is the sum of the energies of repulsion \( V_{\text{rep}} \) (Hogg et al. [8]) and attraction \( V_{\text{attr}} \) (Ho and Higuchi [9]). In eqn (6), \(|r|\) represents the distance of two spherical particles.

### 2.1.2 Flow field

Because of the very fine grid needed for a good resolution of the flow field in the vicinity of the particles, numerical calculations are still inapplicable. Therefore,
analytical expressions for laminar flows are used for the outer annular gap and the conical gap, see hatched areas in fig. 1.

2.2 Limiting trajectories

With eqns (3)–(5) limiting trajectories can be determined. They define a capture cross section upstream from the collector particle through which all trajectories of smaller particles terminate on the surface of the collector particle. In analogy to Higashitani et al. [10], all limiting trajectories end at the rear stagnation point of the collector particle. Assuming a circular capture cross section, limiting trajectories have the radial distance $y_c$ from the streamline of the stagnation point.

2.3 Coagulation efficiency

The coagulation efficiency is defined to be the ratio of curvilinear particle flux $J$ to that of rectilinear particle flux $J_S$ that is given by Smoluchowski [3]. For circular capture cross sections, it can be shown that the coagulation efficiency corresponds to the ratio of the capture cross section and the collision cross section

$$\alpha = \frac{J}{J_S} = \left( \frac{y_c}{a_1 + a_2} \right)^2.$$  (7)

with $a_\alpha$ being the radius of particle $\alpha$.

3 Macroscopic model

For separation apparatuses, a continuous alteration of the particle spectrum takes place as large particles are removed. Thus, a separation coefficient needs to be included when describing the particle interactions by population balances. It gives local information about whether a particle of mass $m$ is already settled out at a given place or not. The combination of both coefficients—the coagulation efficiency and the separation coefficient—is called the integral coagulation efficiency. Based on the investigations of Loeffler [11], the integral coagulation efficiency is modelled in dependence on apparatus geometry, local flow field, particle combination (species and size) and liquid properties.

3.1 Trajectories and particle velocities

Applying the method of Euler–Lagrange, particle trajectories are calculated by integrating the momentum equation on a spherical particle. In order to obtain the velocity components of the flow field in a single gap of a disc stack centrifuge, the commercial CFD tool FLUENT has been used, Breitling et al. [12]. Several assumptions have been made:

- the steady flow is rotationally symmetric,
- the liquid properties are constant, and
• the influence of the gravitational force is negligible compared to the centrifugal force.

The dimensionless equations of particle motion in cylindrical co-ordinates are then given by

\[
\frac{dU_s}{dT} = \frac{1}{1 + \frac{1}{2}(1 - \Delta)} \cdot \left[ 18 \frac{Re}{St} (U_l - U_s) - \frac{\partial P}{\partial X_s}(1 - \Delta) + \right.
\]

\[
Re \cdot (X_s + 2V_s) \left. \right] \tag{8}
\]

\[
\frac{dV_s}{dT} = \frac{1}{1 + \frac{1}{2}(1 - \Delta)} \cdot \left[ 18 \frac{Re}{St} (V_l - V_s) + Re (Y_s - 2U_s) \right] \tag{9}
\]

\[
\frac{dW_s}{dT} = \frac{1}{1 + \frac{1}{2}(1 - \Delta)} \cdot \left[ 18 \frac{Re}{St} (W_l - W_s) - \frac{\partial P}{\partial Z_s}(1 - \Delta) \right] \tag{10}
\]

\[
\frac{dX_s}{dT} = Re \cdot U_s \tag{11}
\]

\[
\frac{dY_s}{dT} = Re \cdot \frac{V_s}{X_s} \tag{12}
\]

\[
\frac{dZ_s}{dT} = Re \cdot W_s \tag{13}
\]

with the dimensionless variables

\[
T = \frac{\mu t}{\varrho_l b^2}, \quad \Delta = 1 - \frac{\varrho_l}{\varrho_s}, \quad P = \frac{p}{\mu \omega}, \tag{14}
\]

\[
St = \frac{\varrho_s d^2 \omega}{\mu}, \quad Re = \frac{\varrho_l b^2 \omega}{\mu}, \tag{15}
\]

\[
U_{l/s} = \frac{u_{l/s}}{\omega b}, \quad V_{l/s} = \frac{v_{l/s}}{\omega b}, \quad W_{l/s} = \frac{w_{l/s}}{\omega b}, \tag{16}
\]

\[
X_s = \frac{x_s}{b}, \quad Y_s = y_s \quad \text{and} \quad Z_s = \frac{z_s}{b} \tag{17}
\]

that depend on time \( t \), pressure \( p \), liquid and solid densities \( \varrho_l \) and \( \varrho_s \), particle diameter \( d_s \), and the angular velocity \( \omega \).

### 3.2 Adhesion constraint

The so-called critical impact velocity \( v_{crit} \) of the smaller particle (superscript \( f \)) characterizes the transition between adhesion and rebound. If the magnitude of the real particle velocity \( v_{f} \) exceeds \( v_{crit} \), coagulation will not take place. Therefore, it is necessary to prove in advance the adhesion constraint when calculating the integral coagulation efficiency. The critical impact velocity can be derived by the
conservation equations of momentum and energy. Its dimensionless and non-linear conditional equation is given in dependence on the impact parameter $k$

$$\lambda^3 \psi \left[ k^2 (1 + \lambda^3 \psi) - \lambda^3 \psi \right] \cdot V_{crit}^2 - \lambda^3 \psi \cos \varphi \cdot V_{crit} +$$

$$\left[ k^2 (1 + \lambda^3 \psi) - 1 \right] - \frac{12}{\pi} \frac{(1 + \lambda^3 \psi)}{dC^3 \frac{\rho C v C^2}{2}} \cdot \Delta E_A = 0. \quad (18)$$

The dimensionless parameters are defined by

$$V_{crit} = \frac{v_{crit}}{v_C}, \quad \lambda = \frac{d_f}{d_C} \leq 1 \quad \text{and} \quad \psi = \frac{\rho_f}{\rho_C} \quad (19)$$

where the superscript $C$ represents the collector particle. The angle between the particle velocity vectors $\varphi$ is obtained by the definition of the scalar product. In order to determine the difference of repulsive and attractive energies before and after the impact $\Delta E_A$, the following assumptions have been made:

- the particle diameters are much bigger than the size of deformation due to the impact and
- the deformation depths of each particle are equal.

In analogy to Dahneke [13], Hiller [14], Krupp [15], Tsouris and Yiacoumi [16], $\Delta E_A$ can be derived. Together with eqn (18), the critical impact velocity can now be calculated. The necessary adhesion constraint is then given by

$$|v_f| < v_{crit}. \quad (20)$$

### 3.3 Integral coagulation efficiency

Only if eqn (20) is true, coagulation of two particles will take place. The integral coagulation efficiency can be determined as a function of the modified Stokes number

$$\tilde{St} = \frac{\rho_f d_f^2 |v_f| \cdot v_f^2}{18 \mu d_C \left( v_C - v_f \right)^2} \quad (21)$$

In analogy to Loeffler [11], the integral coagulation efficiency is defined by

$$\alpha^* = \left( \frac{\tilde{St}}{St + \gamma_1} \right)^{\gamma_2} \quad (22)$$

with $\gamma_1 = 0.65$ and $\gamma_2 = 3.7$. When particles have diameters less than 1 $\mu$m, perikinetic interactions are dominant compared to orthokinetic interactions. For
small Peclet numbers \((Pe < 1)\), the integral coagulation efficiency is determined by Russel, Saville and Schowalter [17]

\[
\alpha^\star = 2.52 \cdot Pe^{-2/3}
\]

(23)

where the Peclet number is defined by

\[
Pe = \frac{6\pi \mu d_f C_f |v_C - v_f|}{k_B T}
\]

(24)

with the absolute temperature \(T\) and the Boltzmann’s constant \(k_B\).

4 Results

For a flow rate of \(\dot{V} = 117\) l/h and an angular velocity of \(\omega = 173\) \(s^{-1}\), the (integral) coagulation efficiencies have been calculated in a single gap of a disc stack centrifuge. The geometry corresponds to that given in table 1 and the suspension consists of a glycerine/water-mixture \((\varrho_l = 1156\) kg/m\(^3\), \(\mu = 0.01\) Pas) with glass spheres \((\varrho_s = 2465\) kg/m\(^3\)). For a mean porosity of 40\% the density of the resulting agglomerates is \(\varrho_s = 1940\) kg/m\(^3\) and the concentration of the coagulant agent (NaOH and CaCl\(_2\)) corresponds to 1 g/l.

![Figure 3: Integral coagulation efficiency \(\alpha^\star\) in dependence on particle diameters at a defined position in the annular gap.](image)

In fig. 3, the integral coagulation efficiency is shown in dependence on particle sizes at a defined position in the annular gap. For a combination of small particles with different sizes the integral coagulation efficiency has maximum values as the relative velocity is high. Due to the additional precipitation of larger particles in the...
centrifuge this behaviour decreases, which means in turn that the integral coagulation efficiency becomes lower. For particles with same diameters, the coagulation efficiency vanishes since the critical impact velocity is very small. This behaviour corresponds to experimental investigations.

Comparing the microscopic and macroscopic models directly becomes very complex as there are too many parameters influencing the efficiencies respectively. Therefore, the local particle size distributions calculated by the method of population balances with different models for the (integral) coagulation efficiency are regarded. An example of these distributions at radius $r = 59$ mm in the conical gap shows fig. 4. They fit well with the experimentally gained mass distribution at the same position in the gap. Differences between the calculated distributions appear only at large particles. For particles with $d_s > 10 \, \mu m$, the distribution determined with the macroscopic model is displaced towards smaller particles as the model contains an additional separation coefficient.

In summary, both methods are suited for predicting the (integral) coagulation efficiency in dependence on flow pattern, apparatus geometry, liquid and solid behaviour. Whilst the macroscopic model only considers particles that have not been separated at a given position, the microscopic model can be used only for analytical flow patterns.

References


