Simulation of acoustic particle agglomeration in poly-dispersed aerosols

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Abstract
This report presents application of the MD for the simulation of acoustic agglomeration of poly-disperse aerosol particles. The conventional time-driven MD approach was applied and in-house developed MD code was modified for simulation purposes. The aerosol is assumed to be a system of dispersed spherical fluid particles while the agglomeration may occur between initial smaller particles sequentially forming larger particles. The modelled processes include the agglomeration due to the orthokinetic and acoustic wake mechanisms. Orthokinetic agglomeration refers to the agglomeration due to direct collisions between particles that are entrained at different velocities in the oscillatory motion of the sound field. Acoustic wake mechanisms are those that produce particle interactions through the surrounding medium because of hydrodynamic forces and the asymmetry of the flow field around the particle. It is assumed that the particles collide and agglomerate due to the interactions induced by sound waves. The aggregates formed during the agglomeration process were characterised as aggregates with a different radius to estimate the average radius of the primary particles in individual aggregates. The MD model was validated by comparison against the available analytical solutions. Finally, interaction process of two and four particles investigated and presented.

Keywords: aerosol, acoustic agglomeration, acoustic wake effect, hydrodynamic particle interactions, orthokinetic effect.

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### Nomenclature

\[ a_i = \{a_{xi}, a_{yi}, a_{zi}\} \]  
Vector of the translational acceleration of \( i \) particle  
\[ d = \{d_x, d_y, d_z\} \]  
Vector of normalized sound direction  
\[ F_i = \{F_{xi}, F_{yi}, F_{zi}\} \]  
Vector of resultant forces of particle \( i \) acting in the centre of particle  
\[ F_{di} \]  
Result fluid force of particle \( i \) acting in the centre of particle  
\[ F_{gi} \]  
Gravity force of particle \( i \) acting in the centre of particle  
\[ f \]  
Frequency of sound  
\( i, k \)  
Subscript notation of particle index  
\( l \)  
Slip of the particle in the Oseen regime  
\( m \)  
Subscript notation of quantity belonging to surrounding medium  
\( m_i \)  
Mass of \( i \) particle  
\( \mu_m \)  
Dynamic viscosity  
\( \nu_m \)  
Kinetic viscosity  
\( \omega \)  
Angular frequency of sound  
\( p \)  
Subscript notation of quantity belonging to particle  
\( Re_{pi} \)  
Reynolds number of particle \( i \)  
\( R_i \)  
Radius of particle  
\( \rho \)  
Fluid or particle density  
\( r \)  
Inter-particle distance  
\( \sigma_g \)  
Geometric standard deviation  
\( t \)  
Time  
\( s \)  
Subscript notation of quantity belonging to sound  
\( \theta_k \)  
Direction of sound with respect to plane \( O_{xy} \)  
\[ u_i = \{u_{xi}, u_{yi}, u_{zi}\} \]  
Vector of the translational velocity of \( i \) particle  
\( U_{s0}, U_{x0} \)  
Amplitude of sound velocity  
\( u_s \)  
Acoustic velocity  
\( u_{rel,i} \)  
Vector of relative velocity between medium and particle  
\( u_m \)  
Vector of medium velocity  
\( u_{pi} \)  
Vector of particle velocity  
\( x_i = \{x_i, y_i, z_i\} \)  
Vector of the translational position of \( i \) particle

### 1. Introduction

Acoustic agglomeration of dispersed aerosol particles is a process in which intense sound waves produce relative motions and collisions between initial small particles sequentially forming larger particles. It is observed that the agglomeration can significantly shift the particle size distribution of an aerosol from smaller to larger sizes in a short time of the order of 1 s. Acoustic agglomeration has a potential to be used in air pollution control. Enhancement of the efficiency of conventional particle filtering devices, which are inefficient for retaining smaller particles in a range of micrometers, is a primary manifest of acoustic agglomeration.

Aerosol is particulate media, therefore, particle-based approach is natural numerical technique could be applied for its simulation. Development of the MD for aerosol particles follows formally the conventional path, and it is focussed on evaluation of all available particle forces including binary interactions with neighbour partners, particle–fluid interaction and the external field induced forces. Detailed classification of particle forces occurring in fluid may be found in review papers [1] and [2]. Concerning acoustics induced forces, the reviews of Xiang et al. [3], Li et al. [4], Shuai et al. [5] may be pointed out.

The process of acoustic agglomeration is governed by various the particle-fluid and the particle-particle interactions, and several approaches for acoustic agglomeration have been formed. The orthokinetic collisions and the hydrodynamic acoustic wake effect are dominant first-order effects leading to the
agglomeration of poly-dispersed particle systems. Theoretical aspects of various agglomeration mechanisms are discussed in [6]-[9].

Orthokinetic interactions refer to the agglomeration due to direct collisions between particles that are entrained at different velocities in the oscillatory motion of the sound field. Particles with different sizes are entrained differently by motion of the medium because of the differences in particle inertia. The earlier investigations on orthokinetic collisions date back to the contribution of Mednikov [10]. Important contribution of Dong et al. [11] with respect to the separate and combined effects of orthokinetic collision may be emphasised. Nevertheless, the orthokinetic collision mechanism is able to model particle collisions that occur due to the different particle entrainments; it does not explain agglomeration for particles with identical or similar sizes.

Hydrodynamic mechanisms are those that produce particle interactions through the surrounding medium because of hydrodynamic forces and the asymmetry of the flow field around the particle. The wake, termed the acoustic wake, leads to a pressure reduction in the area behind the leading particle. If the other particle follows this acoustic wake, it experiences a drag reduction and moves at an accelerated speed towards the leading one. It was observed that the acoustic wake is the first order effect causing, generally, dominant hydrodynamic agglomeration mechanism. A theory to describe the acoustic wake effect based on Oseen flow fields was first proposed by Pshenai-Severin [12] for two same-sized particles aligned along the direction of the sound wave. Dianov et al. [13] extended the theory to include the interactions between differently sized particles and derived an analytical solution. The acoustic wake effect combined with gravitationally settling particles forms the characteristic tuning-fork patterns first discovered by Hoffman and Koopmann [14,15].

In presented work, the MD methodology were adopted to for simulation of acoustic agglomeration of aerosol particles and the conventional MD code is adopted for simulation purposes. In Section 2, methodology and basic relations of the particles interactions method applied to the dynamic behaviour of aerosols is described. In the section 3 numerical results are presented.

2. Simulation methodology and basic relationships

The particles of spherical shape with radius $R_i$ embedded into the surrounding incompressible medium are considered. The medium is characterised by the density $\rho_m$, the dynamic and kinematic viscosities of the medium $\mu_m = \nu_m \rho_m$ and $\nu_m$, respectively. The subscript $m$ will be used for indication of the medium parameters.

External excitation presents the sound field having a constant initial sound intensity with the maximum at the surface of the distributor. The sound source is characterized by the sound velocity amplitude, $U_{0x}$, and the frequency, $f$. Thus, the sound attenuation of the distributor is neglected. Several main assumptions will be introduced in considering the behaviour of aerosol particles. Their formulations defined regarding given parameters are as follows.

The spatial variation of acoustic wave is neglected. In a series of our simulation experiments, the acoustic wave propagates horizontally while direction of sound with respect to plane $Oxy$ is defined by angle $\theta_z$. Finally, in-plane motion of the sound wave in time $t$ with $\theta_z = 0$ is described by a sinusoidal acoustic velocity $u_z = u_z(t)$ in a form

$$u_z(t) = U_{0x} \sin(\omega t),$$  \hspace{1cm} (1)

where $\omega$ is the angular frequency, $\omega = 2\pi f$.

Agglomeration mechanism is driven by binary coalescence of particles after collision, and it is considered in the following manner. Two particles $i$ and $k$ collide upon the condition that particles overlap occur, i.e. when the inter-particle distance $r_{ik}(t)$ between surfaces of two approaching particle drops to zero. Consequently, contact and short range attractive forces are not taken into account. When this condition is
satisfied, two particles are merged into the one bigger particle. Assuming that particle $k$ disappears from the system, while characteristics of the new modified particle $i$ is obtained regarding conservation laws

Lagrangian approach and molecular dynamic methodology was applied for simulation of the dynamic behaviour of aerosol particles. The particle interactions offers a direct way to study the state of particulate solid numerically by computing the motion and interactions of individual particles.

The translational particle’s motion is described in a Cartesian framework of classical mechanics and obeys Newton's second law. Here, axis Oy points the vertical direction. An arbitrary particle $i$ in 3D is treated as a solid body with mass $m_i$. It’s motion in time $t$ is described in the global Cartesian frame of reference and characterized by the position vector of the particle mass centre $x_i$, the translational velocity $u_i = \dot{x}_i = dx_i / dt$ and the acceleration $a_i = \ddot{x}_i = \dddot{x}_i$. Governing equations of the particle can be written vector form as

$$m_i \ddot{u}_i = F_i(t).$$  \hspace{1cm} (2)

Here, vector $F_i$ presents the resultant force acting in the centre of the particle. In summary, resultant force of an arbitrary particle $i$ comprises several components

$$F_i = F_{di} + F_{bi} + F_{gi}.$$ \hspace{1cm} (3)

The gravity force $F_{gi}$ and the buoyancy force $F_{bi}$ will be taken into account where they are appropriate. The notation $F_{di}$ stands for the drag force. The expression of this acoustically induced force reads, see [6]:

$$F_{di} = 6\pi\mu_i R_i \left(1 + \frac{3}{16} Re \right) u_{rel,i}.$$ \hspace{1cm} (4)

A non-dimensional parameter, $Re$, is the Reynolds number for particle $i$. It is expresses in terms of properties of a surrounding medium as follows:

$$Re = 2R_i \rho_m |u_{rel,i}| / \mu_m.$$

It is obvious that drag force as well as Reynolds number [6, 13] depends on velocities. Here, $u_{rel,i}$ stands for the relative velocity [7] between the velocities of medium $u_m(t)$ and the particle (slip-flow) velocity $u_{p,i}$,

$$u_{rel,i}(t) = u_m(t) - u_{p,i}(t)$$ \hspace{1cm} (6)

Since aerosol particles are partially entrained into the oscillating motion of the medium, the velocity of an isolated particle $u_{p,i}(t)$ in the interactions calculations is obtained numerically by solving (2).

If we assume a synchronous motion of medium with the propagation of the sound, the disturbance velocity is the velocity of medium due to acoustic motion (1)

$$u_m(t) = u_s(t)$$ \hspace{1cm} (7)

This expression (7) reflects conditions of orthokinetic agglomeration, neglecting, however, inter-particle effects.

The particle interactions simulation methodology comprises time integration of equation (1) and the explicit Verlet integration scheme is used. Positions $x_i$ and velocities $u_i$ of each particle are determined incrementally using small time steps.
3. Numerical results

A series of numerical tests were performed to validate the numerical model and to demonstrate the method. The basic data used in our simulations are characterized in the following way. The monochromatic sound wave is characterized by an amplitude velocity $U_{\text{\textit{in}}}^0$ and a frequency $f$. The surrounding medium is defined by density $\rho_m$ and dynamic viscosity $\nu_m$. Particle properties are characterized by density $\rho_p$ and by radius $R$. The summary of data value applied in our simulations is given in Table 1, where each of the lines are relevant to a particular sample.

<table>
<thead>
<tr>
<th>Characterization of sample</th>
<th>Sound data</th>
<th>Medium data</th>
<th>Particle data</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$U_{\text{\textit{in}}}^0$ m/s</td>
<td>$f$ kHz</td>
<td>$\rho_m$ kg/m$^3$</td>
</tr>
<tr>
<td>Sample 1</td>
<td>1.0</td>
<td>100.</td>
<td>1.2</td>
</tr>
<tr>
<td>Sample 2</td>
<td>1.0</td>
<td>200.</td>
<td>1.2</td>
</tr>
<tr>
<td>Sample 3</td>
<td>1.0</td>
<td>200.</td>
<td>1.2</td>
</tr>
</tbody>
</table>

The first computations are aimed to validate performance of the elaborated methodology. The data for these tests are given in Table 1.

Sample 1. The testing problem denoted hereafter as Sample 1 comprises validation of numerical results against analytical solution. The interaction between two identical spherical particles $i$ and $k$ during the approach motion was simulated numerically, and the numerically obtained variation of the relative inter-particle velocity $u_{12}$ along inter-particle distance coordinate $r$ was compared with the analytical solution presented by Dianov et al. [13]. More definitely, analytical expression for the acoustically induced wake is given by formula:

$$\bar{u}_{ik}(r) = \frac{2}{\pi} \left( \frac{3RIU_{\text{\textit{in}}}^0}{3r} \left( 1 + \frac{RIU_{\text{\textit{in}}}^0}{\pi \nu} \right) - \frac{1}{r^2} \left( \frac{6R \nu}{\pi} + \frac{9R^2IU_{\text{\textit{in}}}^0}{16} \right) \right)$$

(8)

Simulation results are presented in figure 1.

Fig. 1. Variation of the relative inter-particle velocity $u_{12}$ during approaching distance – comparison of numerical results against analytical solution.
3.1. The agglomeration of two differently-sized particles

Agglomeration of two differently sized particles having radii $R_1$ and $R_2$ will be illustrated by considering effect of the relative size ratio $= R_1/R_2$. A set defined by considering four cases $= 1.0; 1.5; 2.0; 4.0$ was analysed. Figure 2 shows the particle trajectories.

![Fig. 2. Agglomeration patterns for binary interaction of differently sized particles (initial distance 20 μm, initial angle 30°)](image)

3.2. The Multi-particle sequential agglomeration mechanism.

The multi-particle sequential agglomeration mechanism is based of superposition of all interactions onto particle. Each particle interacts with other particles throw acoustic wake force. Additionally, each particle could collide throw orthokinetic induced collision. All other hydrodynamic effects was neglected. New one particle is formed after collision from old two’s by calculating of radii of new particle from volume of old particles. So, collisions induced agglomeration process always is going pairwise between come nearest particles.

3.3. The Agglomeration of multi-particle system.

Agglomeration of fourth equivalent sized particles having radii $R_1$ will be illustrated by considering effect of serial pair particle convergence. A set two defined configurations was analyzed. First set represents random generated configuration, second shows initially mirror quasi-symmetric configuration. Both initial configurations are taken in Figure 3 and show the particle trajectories before and after agglomerations. Left side picture shows finally agglomeration of four particles, the opposite right side picture shows divergence of two agglomerated particles.
4. Concluding remarks

Application of the MD for simulation of acoustic agglomeration in poly-dispersed aerosols was proposed. It is assumed that the particles collide and agglomerate due to the interactions induced by sound waves. The aggregates formed during the agglomeration process were characterised as aggregates with a different radius to estimate the average radius of the primary particles in individual aggregates. Comparison of obtained numeric results with theoretical results of other authors shows good agreement. Finally, interaction process of four particles shows that agglomeration is going in numeric simulation pairwise between come nearest aerosol particles.

References