Simulation of attractive motion of silica microparticles in aerosol under acoustic excitation

Rimantas Kačianauskas[1], Irina Kačinskaja[2], Algirdas Maknickas[3], Darius Markauskas[4], Jerzy Rojek[5]*

[1,2,3,4] *Institute of Mechanics, Vilnius Gediminas Technical University,*
J. Basanavičiaus Str. 28, 03224 Vilnius, Lithuania
e-mail: rimantas.kacianauskas@vgtu.lt [1], irina.kacinskaja@vgtu.lt [2], algirdas.maknickas@vgtu.lt [3], darius.markauskas@vgtu.lt [4]

[5] *Institute of Fundamental Technological Research, Polish Academy of Sciences,*
Pawińskiego ul. 5B, 02-106 Warszawa, Poland,
e-mail: jrojek@ippt.gov.pl

Abstract

Numerical simulation of the attractive motion of dry silica microparticles in incompressible media under acoustic excitation is considered. The silica microparticles are spheres of the diameter are varying between 5 and 10 μm. A moving monochromatic sound wave initiates attraction forces between particles, resulting from the oscillatory motion of the media. The effect of orthokinetic and acoustic wake hydrodynamic interaction mechanisms, as well as gravity and buoyancy forces, is taken into account. The conventional time-driven Discrete Element Method (DEM) is applied for simulation purposes, and the developed in-house DEM code was modified for simulation purposes. Binary attraction of particles differently located with respect to the direction of the sound wave is considered numerically and agglomeration time is investigated. The results are compared with the analytical solutions, and the experimental data described in the literature. The simulation of a 2D polydispersed particle system is also demonstrated.

Keywords: DEM, silica microparticles, acoustic excitation, hydrodynamic interactions, orthokinetic effect, wake effect

1. Introduction

Silica dust is produced during various construction or mining works. Silica dust is formed by tiny particles which can be inhaled into the lungs and cause serious health problems. Silica particles released into the air can form aerosol clouds, systems of particles suspended in the air. Acoustic excitation is used in different devices to manipulate aerosol particles. The purpose of the work is to improve understanding of interparticle and fluid-particle interaction mechanisms under acoustic excitation.

An attractive behaviour of microparticles is observed under action of the acoustic sound wave. This behaviour is governed by various hydrodynamic particle-fluid and particle-particle interactions. It is stated [5], that the orthokinetic collisions and the hydrodynamic acoustic wake are dominant first-order effects causing the agglomeration of polydispersed particle systems. The earlier investigations on orthokinetic collisions were performed by Mednikov [7] and the important contribution was made by Dong et al. [3]. A theory describing the acoustic wake effect based on Oseen flow fields was first proposed by Pshenai-Severin [8]. Dianov et al. [2] extended the theory to include the interactions between particles of different size and derived an analytical solution. A detailed classification of particle forces acting in fluid can be found in the review paper of Deen et al. [1]. As concerns the acoustics induced forces, the paper of Li et al. [5] can be mentioned.

In the paper, attractive motion of silica dust microparticles under acoustic excitation is investigated using the discrete element method (DEM). Dynamic behaviour of the system is described using the Lagrangian approach. The motion of an individual particle is defined according to Newton's laws of classical mechanics. Agglomeration patterns and the influence of particle arrangement on the approaching time is analysed.

2. Problem description

The silica dust microparticles are assumed rigid spheres with the diameters varying between 5 and 10 μm. Generally, the particle assembly is characterised by statistical distribution of the particle diameters, while characterisation of mechanical properties is restricted to their mass density ρ_p only. The particles are dispersed in the air, which is assumed a viscous incompressible medium. The medium is characterized by the density ρ_m, the dynamic and kinematic viscosities of the medium $\mu_m = \upsilon_m \rho_m$ and υ_m, respectively.

External acoustic excitation presents a monochromatic sound wave propagating horizontally in plane *Oxy*. It is described by sinusoidal acoustic velocity $u_s = u_s(t)$ characterized by sound velocity amplitude U_{s0} and frequency f.

A travelling sound wave initiates the attractive forces between the particles, resulting from oscillatory fluid motion. The modelled processes are considered in plane *Oxy* on the scale of the inter-particle distance, while the attractive short-range forces are neglected.

3. A concept of DEM modelling

The conventional DEM approach was modified for simulation purposes. The translational motion of an arbitrary particle p with mass m_p in time t is characterized by the position and velocity vectors of the particle mass centre $\boldsymbol{x}_p(t)$ and $\boldsymbol{u}_p(t)$, respectively, with respect to the Newton's second law.

The governing equation of the particle motion is written in a vector form as follows:

$$m_p \frac{\mathrm{d}\boldsymbol{u}_p(t)}{\mathrm{d}t} = \boldsymbol{F}_{dp} + \boldsymbol{F}_{gp} + \boldsymbol{F}_{bp} \qquad (1)$$

The problem was solved numerically by time integration of the equations of motion (1), where $\boldsymbol{F}_{dp}$ denotes a drag force describing particle-fluid-particle interactions and comprising the

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Stokes force and the so-called Oseen's correction, $\boldsymbol{F}_{gp}$ is a gravity force and $\boldsymbol{F}_{bp}$ is a buoyancy force. The conventional time-driven DEM approach [4] and the in-house developed DEM code were modified for simulation purposes. The detailed description of the DEM acoustic agglomeration model can be found in [6].

4. The numerical results

A series of numerical tests were performed to illustrate attractive motion of microparticles. The silica dust particles characterized by the density $\rho_p = 1500$ kg/m^3 were considered. The air medium at temperature 20° C is characterized by the density $\rho_m = 1.293$ kg/m^3 and the dynamic viscosity $\mu_m = 17.9 \cdot 10^{-6}$ m^2/s. The generated monochromatic sound wave is characterized by the amplitude velocity $U_{s0} = 0.378$ m/s (SPL 135 dB) and the frequency $f = 24$ kHz.

The motion of particles from the position fixed at time instant $t_0 = 0$ is tracked by numerical integration of Eqn (1). Since the oscillation period of the sound is $T_s = 0.042 \cdot 10^{-5}$ s, a very small time step $\delta t = 1.0 \cdot 10^{-7}$ s was used in simulation.

The possible contact between particles was checked at each time step during the simulation. If the contact was found, two particles were assumed to be merged into one bigger particle. The attractive motion during binary interaction of two particles with diameters equal to $d = 5$ μm and $d = 10$ μm, which were located at the initial interparticle distance of 2000 μm. The illustrations of the simulation results in terms of the trajectories of particles in plane *Oxy* are presented in Fig. 1. The graphs demonstrate dependence of the attraction-driven approaching trajectories on sound direction, where the transformation of a straight line into the line of complicated shape can be clearly seen.

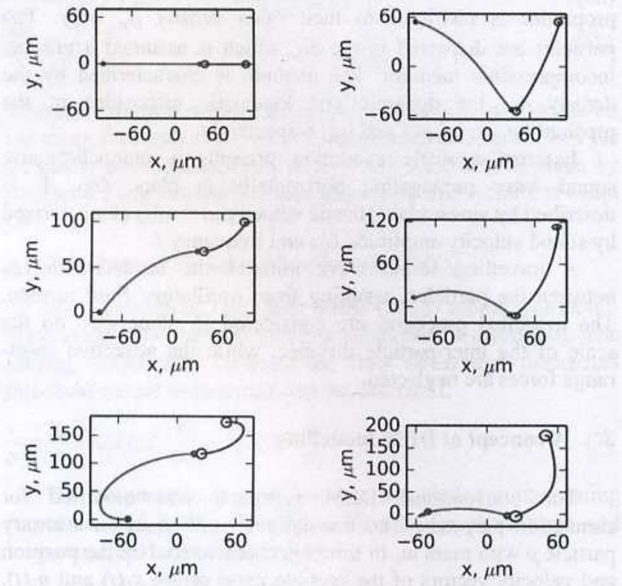

Figure 1: Trajectories of attractive motion of particles of different diameters: $d = 10$ μm (Particle 1) and $d = 5$ μm (Particle 2) without (left column) and with (right column) vertical forces for different direction of the sound

In the limit, when inclination line became perpendicular to sound direction, the attractive behaviour is transformed into repulsion. The line positions illustrate different contribution of the inclination angle (0°, 30° and 60°) between the initial interparticle line and the horizontal direction of the sound. This effect is illustrated by the increase in the agglomeration time. In particular, under the increase of the inclination angle from 0° to 60°, the agglomeration time increases from 0.039 to 0.163 seconds for interaction of equal 5 μm particles, and from 0.0199 up to 0.0817 seconds for interaction of equal 10 μm particles. The attraction behaviour of the particles of different size is more complicated (see Fig. 1.)

5. Concluding remarks

The results obtained in the present work show that DEM is a proper numerical analysis technique for the case of binary attractive behaviour of particles under acoustic excitation and for evaluation of the contribution of various parameters. It was also observed that binary interactions form the base of collective behaviour of multi-particle systems.

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