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Numerical particle-based analysis of the effects responsible for acoustic particle agglomeration

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ABSTRACT

Numerical particle-based modelling of aerosol particles in an acoustic field is performed, and the influence of the effects, including orthokinetic collision, an acoustic wake effect and mutual radiation pressure effect, responsible for the particle agglomeration is analyzed. The standard discrete element method is modified to take into account the drag force of the gas obtained using Oseen's solution and the mutual radiation pressure force. Numerical modelling of the agglomeration of two identical particles in a strong acoustic field is performed, and the results are compared with the available analytical solution and the data obtained in the experiments described in the literature. Finally, the simulation of a 2D polydispersed particle system at various sound frequencies is performed. The obtained results show that the major agglomeration mechanism is the acoustic wake effect, while orthokinetic collision plays an insignificant role.

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1. Introduction

Acoustic agglomeration of dispersed aerosol particles is a process when intense sound waves produce relative motions and collisions between the initial small particles sequentially forming larger particles. Larger particles can be more easily caught using conventional particle filtering devices, and, therefore, acoustic agglomeration is used to significantly enhance the removal rate of the micron size particles [\[1–3\]](#page--1-0).

The process of acoustic agglomeration is governed by various particle–fluid and particle–particle interactions, and several approaches to acoustic agglomeration have been developed. Theoretical aspects of various agglomeration mechanisms are discussed in $[4-7]$. 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. The particles of various sizes are entrained differently by the motion of the medium because of the differences in particle inertia. The earlier investigations into orthokinetic collisions date back to the contribution of Mednikov $[8]$. The important contribution of Dong et al. $[9]$, relating to separate and combined effects of orthokinetic collision, may be also mentioned. Nevertheless, the orthokinetic collision mechanism is able to model particle collisions occurring due to different particle entrainments, but it does not explain the agglomeration of particles of the same or similar size.

Aerosol particles not only interact with the ambient gas, but the interaction between the particles in the gas can be observed. According to the Oseen's solution, an asymmetric flow field is formed around the moving particle. If two particles are in the line with the flow field, then, the drag reduction is less significant for the leading particle, and, as a result, the 'tail' particle moves at an accelerated speed towards the leading one $[10]$. This hydrodynamic interaction is called ''acoustic wake effect'' (AWE) [\[4\].](#page--1-0) The significance of this effect for the agglomeration of particles was studied in $[4,11,6,9,12]$ by using the analytical and numerical methods and was experimentally verified in [13-15].

Two nearby particles exert forces on each other because their scattered waves nonlinearly interact with the incident acoustic wave. This is known as ''mutual radiation pressure effect'' (MRPE), the significance of which is pointed out by Gonzalez and Gallego-Jurez [\[15\]](#page--1-0). The analytical solution for MRPE force was derived by Song [\[16,5\].](#page--1-0) While the experimental and numerical results in [\[17,13\]](#page--1-0) fail to provide the direct evidence to support the Song's hypothesis of scattering interaction as an effective refill mechanism of the emptied agglomeration volumes, the authors in [\[15\]](#page--1-0) suggest that MRPE is behind a repulsion effect observed in combination with the attraction exerted by the AWE.

As noted by Zhang et al. [\[12\],](#page--1-0) the conclusions drown in the cited works about the role of the agglomeration effects do not agree with

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each other and, sometimes, even contradict one another. Therefore, a more comprehensive study of the effects responsible for acoustic particle agglomeration is still needed.

In the past, the particle agglomeration was numerically modelled by many researchers (e.g. $[8,5,4,18,12]$). The well-known Smoluchowski equation can be used to solve the discrete particle or cluster dynamic equation [\[16\]](#page--1-0). As an alternative method for the simulation of acoustic agglomeration, the direct simulation Monte Carlo method was applied by Sheng and Shen [\[18\].](#page--1-0)

Aerosol is particulate medium, therefore, the particle-based approach is a natural numerical technique, which could be applied to its simulation [\[19\]](#page--1-0). The development of the discrete element method (DEM) for aerosol particles follows formally the conventional path, and is focused on the evaluation of all available particle forces, including binary interactions with the neighbouring partners, particle–fluid interaction and the external field induced forces. A detailed classification of particle forces occurring in fluid may be found in the review papers [\[20,21\].](#page--1-0) Concerning the acoustics induced forces, the reviews of [\[15,22–24\]](#page--1-0) may be mentioned.

In the present work, the DEM methodology was adopted for simulating acoustic agglomeration of aerosol particles, and our in-house DEM code [\[25,26\]](#page--1-0) was changed for simulation purposes. In Section 2, the methodology and basic relations of the particle interactions applied to the dynamic behaviour of aerosols is described. In Sections [3](#page--1-0) and [4,](#page--1-0) the obtained numerical results are presented.

2. A theoretical model

The model presented below follows the DEM methodology. Three mechanisms used by other authors and potentially responsible for the acoustic agglomeration are described and incorporated into DEM.

The motion of each aerosol particle is governed by the Newton's Second law:

$$
m\ddot{\mathbf{x}}_p = \mathbf{F}_d + \mathbf{F}_b + \mathbf{F}_g + \mathbf{F}_{MRPE},\tag{1}
$$

where \mathbf{F}_d is the drag force of gas, $\mathbf{F}_b = V_p \rho_g \mathbf{g}$ is the buoyancy force, V_p is the volume of the particle, $\mathbf{F}_g = m\mathbf{g}$ is the gravity force. The drag force can be established in the Oseen regime [\[27\]](#page--1-0) by

$$
\mathbf{F}_d = 6\pi\mu R \left(1 + \frac{3}{16}Re\right) (\mathbf{u}_g - \mathbf{u}_p),\tag{2}
$$

where Re = $2R(|\mathbf{u}_g - \mathbf{u}_p|)/v$ is the Reynolds number, R is the radius of the particle, μ is dynamic viscosity of the fluid ($\mu = v\rho_{\alpha}$), \mathbf{u}_{g} and \mathbf{u}_p is gas and particle velocity respectively. The gas velocity \mathbf{u}_g is expressed as

$$
\mathbf{u}_g = \mathbf{u}_{g,ac} + \mathbf{u}_{g,pv},\tag{3}
$$

where $\mathbf{u}_{g,pv}$ is the perturbation gas velocity and $\mathbf{u}_{g,ac}$ is the vector of gas velocity due to acoustic motion, whose one component is equal to

$$
u_{g,ac} = U_0 \sin(\omega t). \tag{4}
$$

Note, that the spatial variation of acoustic velocity is neglected in Eq. (4).

Particle collisions due to different particle oscillations in the acoustic field (4) (when $u_{g,pv}$ is neglected in Eq. (3)) is called the orthokinetic collision (OC) mechanism $[9]$. However, it is clear that this mechanism can cause the agglomeration of different size particles only, while the agglomeration of similar sized particles cannot be explained by it.

The perturbation gas velocity $u_{g,pv}$ is calculated based on the steady Oseen approximation [\[27\].](#page--1-0) However the use of Oseen approximation may not be necessarily justified in the theoretically strict meaning. Owing to the nonlinear convection term in Navier– Stokes equation, Oseen approximation for oscillatory flow past a sphere can take a completely different form from that for stationary flow. There are no theoretical bases that the flow pattern of oscillatory flow is similar to that of steady flow. Deeper considerations on this theoretical matter can be found in $[28]$. In the present work the perturbation gas velocity $u_{g,pv}$ in the polar coordinates is described in the Oseen regime by the equations presented in $[29]$ at the position of particle *i* generated by particle *k* (Fig. 1):

Fig. 1. The calculation scheme of two particles.

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