Powder Technology 323 (2018) 393–402

Contents lists available at ScienceDirect

Powder Technology

journal homepage: www.elsevier.com/locate/powtec

A new multiple-time-step three-dimensional discrete element modeling of aerosol acoustic agglomeration

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ARTICLE INFO

Article history:
Received 28 August 2017
Received in revised form 10 October 2017
Accepted 19 October 2017
Available online 23 October 2017

Keywords:
Multiple-time-step
DEM
Acoustic agglomeration
Aerosol
Population balance

ABSTRACT

An acoustic agglomeration process, in which high-intensity sound is used to agglomerate particles in aerosols, can be simulated using the discrete element model (DEM). However, the conventional DEM is very time-consuming due to the large difference between the various time scales involved in the modeling. In this paper, a multiple-time-step algorithm is used to speed up the 3D DEM simulation of aerosol acoustic agglomeration, which reduces the computational time by more than one order of magnitude, comparing with the conventional DEM. When the computational domain contains N particles, the computational complexity of the improved DEM simulation is of the order of $O(N)$, by restricting the acoustic wake effect in certain ranges and performing contact detection based on a search grid. The DEM simulation model has been validated by: 1) the analytical solution for the oscillation motion of an isolated particle in a sound field, 2) the experimental result of the agglomeration trajectories of two particles under the mutual effect of acoustic wakes, and 3) the experimental results of acoustic agglomeration of coal-fired fly ash particles. It is found that the agglomeration efficiency obtained from DEM simulation is in good agreement with the experimental results at moderate sound pressure levels, while the simulation overestimates the agglomeration efficiency at a high sound pressure level of 149 dB, due to the breakage of aggregates in the experiment.

1. Introduction

Acoustic agglomeration is an efficient aerosol agglomeration technology in which high-intensity sound is applied to produce relative motions among particles [1]. Once the aerosol particles collide, they are likely to agglomerate together to form larger aggregates due to the van der Waals forces or liquid bridge forces. As a result, the number concentration of the aerosol will be greatly reduced and its particle size distribution (PSD) shifts towards a larger size. This technology has great application potential in the fields of improving removal efficiency of particulate matter in dust filters, recovery of valuable particles or droplets from flue gases, removal of radioactive aerosols in the accidents of nuclear power plants, and airport defogging [2–4].

The most significant mechanisms of acoustic agglomeration are commonly considered to be the orthokinetic interaction and hydrodynamic interactions [5]. According to orthokinetic interaction, aerosol particles with different sizes are entrained into the oscillation of gas medium at different rates, which leads to the relative motion and collision among particles. It has a clear physical meaning, and is thought to be the dominant mechanism for the acoustic agglomeration of dispersed aerosols [6]. The hydrodynamic interactions, produced through the hydrodynamic forces and asymmetry of flow field around the particles, are generally considered to be the dominant mechanisms for the acoustic agglomeration of monodisperse aerosols [7,8]. The proposed hydrodynamic interactions include acoustic wake effect, mutual radiation pressure effect and mutual scattering interaction. The recent theoretical studies have found that only the acoustic wake effect plays the important role in acoustic agglomeration, and the other two effects could be neglected [9–11].

Based on the above mechanisms, the acoustic agglomeration process can be numerically simulated to predict the agglomeration efficiency. Generally, there are two mainly classes of simulation methods: 1) the population balance (PB) modeling, and 2) the discrete-element modeling (DEM).

The PB modeling is a commonly used tool which uses PB equation, also called Smoluchowski's equation or aerosol general dynamic equation, to describe the aerosol dynamic processes. After neglecting the

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https://doi.org/10.1016/j.powtec.2017.10.036
0032-5910/

breakage, nucleation and volatilization, the Smoluchowski's equation is given by [12].

$$\frac{dn(v,t)}{dt} = \frac{1}{2}\int_0^v n\left(v-v',t\right)n\left(v',t\right)K\left(v-v',v'\right)dv' - n(v,t)\int_0^\infty n\left(v',t\right)K\left(v,v'\right)dv', \quad (1)$$

where $n(v,t)$ is the number density of aerosol particles with volumes of v at time t, and $K(v,v')$ is the agglomeration kernel between two particles of volumes v and v', which is determined by the involved agglomeration mechanisms.

The Smoluchowski's equation cannot be solved analytically unless the agglomeration kernel is constant or a simple function of particle volume [13]. Several methods have been developed to solve the equation numerically, including discrete method (sectional algorithm) [14], moment method [15], Monte Carlo method [16], and so on.

It should be noted that the PB model describes aerosol dynamic behaviors on a macroscopic level, and the application of this model is restricted in many respects. The main two assumptions and restrictions of the model are as follows: 1) The PB equation is a zero-dimensional and macroscopic model, which cannot consider the heterogeneous distribution of aerosol particles. The assumption of the equation is that the aerosols are well-mixed and homogeneously distributed [17,18]. In an acoustic agglomeration process, however, this assumption is not satisfied, because the micron-sized particles are impossible to be distributed homogeneously in a time scale of one acoustic cycle under the effect of sound, Brownian diffusion or turbulent diffusion. 2) The agglomeration kernel need to be obtained prior to solving the PB equation. For orthokinetic interaction mechanism, the agglomeration kernel can be derived by introduction of the conception of agglomeration volume, which is assumed to be completely refilled in one cycle of the acoustic wave [19]. However, it is difficult to derive the agglomeration kernel of the hydrodynamic interactions, which are more complex than the orthokinetic interaction [20]. As a result, the hydrodynamic interactions are unlikely to be included in the PB modeling. In addition, it is hard to obtain the total agglomeration kernel when several mechanisms act simultaneously, because combining these individual agglomeration kernels by summary or weighted averaging both lack theoretical foundation. Therefore, the PB model is more like an empirical model, which would not represent the real physical nature of aerosol acoustic agglomeration.

On the other hand, DEM is a particle-based direct numerical simulation method, which is on a microscopic level. The velocity and trajectory of each particle in an aerosol are solved according to the all the forces acting on them using Newton's second law. Hence, all mechanisms responsible for agglomeration can be conveniently included in the model. Moreover, the coupling interaction between particles and fluid can also be included. Therefore, the DEM method describes the real physical process of aerosol particles, and is capable of avoiding all the assumptions of the PB model.

The DEM method was originally developed by Cundall and Strack [21] to simulate the granular flow in rock mechanics, and now it has been also applied to solve aerosol dynamics problems. Recently, the exploratory applications of DEM to acoustic agglomeration processes were carried out by some researchers [9,22,23]. The main shortcoming of DEM is that it is computationally expensive and therefore not suitable for a large number of particles, especially for simulating aerosols. The sizes of aerosol particles are much less than that in granular flow, and usually cover a wide range of several orders. As a result, the time scales associated with several involved physical processes in an aerosol dynamics problem can vary over an extremely wide range. In particular, a very small time step is usually required to detect the collision between particles, which makes the simulation particularly time-consuming.

A multiple-time-step algorithm for DEM has been proposed by Marshall [24] to speed up the DEM simulation of aerosol dynamics, which uses three different time steps, i.e. the fluid time step, the particle time step and the collision time step. The computational tasks, such as updating fluid flow, solving particle motion, collision detection and identifying a list of neighboring particles, are performed at their corresponding time steps. By this method, it is possible to carry out the most time-consuming computational tasks at the longest time step, i.e. the fluid time step. The multiple-time-step algorithm can dramatically reduce the computational time required for the DEM simulation of aerosols [25,26]. However, the application of this algorithm to simulate an aerosol acoustic agglomeration process has not been published yet.

In this paper, a DEM method for aerosol acoustic agglomeration using multiple-time-step algorithm is presented, and the numerical agglomeration models and their implementation in the simulation are discussed. The simulation results are verified by the analytical solutions and experimental results. The current study aims to provide an efficient and accurate numerical tool for predicting the agglomeration efficiency of aerosol acoustic agglomeration processes.

2. Algorithm and theoretical models

2.1. Multiple-time-step DEM algorithm

The motion of aerosol particles suspending in the gas medium is governed by the all the forces acting on them, which is given by Newton's second law:

$$\frac{du_p}{dt} = \sum F, \quad (2)$$

where u_p is the particle velocity and F is the total force acting on the particle.

The aerosol dynamic behavior can be described by integrating the motion equations for every single particle. It is essential to choose a proper time step for Eq. (2) based on the time scales that associated with the involved physical processes. In an aerosol acoustic agglomeration process, the mainly time scales include the flow time scale, the particle aerodynamic response time scale and the collision time scale, which can be described as follows.

(1) **The fluid time step**: In an acoustic agglomeration process, the fluid is oscillating at the acoustic frequency, so the time step should be small enough to resolve the sinusoidal oscillation, given as

$$\Delta t_f = k_f T_a, \quad (3)$$

where Δt_f is the fluid time step, T_a is the acoustic period, and k_f is a coefficient with a value much less than unity.

(2) **The particle time step**: It represents the response time of a particle to the fluid motion, and is determined by the particle relaxation time, given by

$$\Delta t_p = k_p \tau_p = k_p \frac{\rho_p d^2}{18\mu_g}, \quad (4)$$

where Δt_p is the particle time step, τ_p is the particle relaxation time, ρ_p is the particle density, d is the particle diameter, μ_g is the dynamic viscosity of fluid, and k_p is a coefficient with a value less than or equal to 1.

(3) **The collision time step**: In order to identify and resolve particle collision, the collision time step is given as.

$$\Delta t_c = k_c \frac{d_{min}}{u_c}, \quad (5)$$

where Δt_c is the collision time step, d_{min} is the minimum particle diameter in an aerosol, k_c is a coefficient with a value much less