Study on the Influence of Electrostatic Force on Collision Efficiency between Micro-Particle

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Abstract. This paper is mainly about the impact of electrostatic forces on the collision efficiency, which collision is caused by the internal forces between micro-particles. The Fourth-order Runge-Kutta method is used to solve the dynamical equations of the micro-particle collision. Studies have shown that the micro-particles with the same charge have the same initial velocity, the larger the volume of the particles, the more the charge amount, and the different particle size has a greater impact on the repulsion effect during the collision. That is, the repulsion effect exhibited in the collision between particles is related to the particle size; Micro-particles with different kinds of charges have the same initial velocity, the smaller the volume, the less the charge amount, and the smaller the particle size, the more attractive the collision effect during the collision.

1. Introduction
A colloidal dispersion formed by suspending solid or liquid micro-particles in air is called an aerosol. The cloud of nature, the soot produced by kitchen cooking, the soot produced by industrial production, and the anxiety PM 2.5 are all examples of aerosols [1]. The related “purification” and “dust removal” industries derived from this and the particle collision research with more in-depth exploration principles are also receiving more and more attention.

At present, researchers at home and abroad have done a lot of research on particle collision, and have achieved many results in theoretical analysis, numerical simulation and experimental verification [2]. Zhang Wenbin and others took the lead in abandoning the original macroscopic study of particle agglomeration, studied the phenomenon of particle agglomeration from a microscopic point of view, and proposed the main forces affecting particle agglomeration and rupture as elastic force and van der Waals force [2, 3]; By tracking the virtual particles which are much smaller than the actual number of particles, Zhao Haibo proposed the selection criteria of time step, the judgment criterion of the control volume of the virtual collision partner, the judgment criterion of particle collision occurrence, the selection of virtual collision partner, etc. A complete multiple MonteCarlo algorithm which considers particle collisions has been constituted. The numerical simulation of the micro-particle flow and the coarse heavy particle flow in the ideal working condition is carried out; Zheng Jianxiang studied the effect of repulsive potential energy $U_{\text{max}}$ on the aggregation rate, introduced the capture efficiency $f(\alpha)$ to modify the agglomerated nucleus, and numerically simulated the particle agglomeration process by coupling the CFD with the population equilibrium model, the error between the results and the
experimental results is only 8%; Mahdavi carried out numerical simulation and experimental research on alumina micro-particles. Combined with Brownian motion, thermophoresis, lift, buoyancy, centrifugal force, virtual mass, pressure gradient, van der Waals force and electric double layer repulsive force [4, 5], a new kind of the microparticle slip speed has obtained good results, and the thermophoresis and electrostatic force[6, 7] should be considered more when the nanoparticle research is proposed.

However, this is not the case in real life. In the case of collision and condensation of micro-particles under electric field or application to electrostatic precipitator, the micro-particles are usually charged particles. In the process of collide and separate between the particles, the micro-particles are also charged [8]. At this time, the electrostatic force is no longer a negligible amount, but a physical quantity that has a certain influence on the collision and coagulation of the particles. At the same time, the electrostatic force has a large range of effective influence [9], a wide range of related phenomena, technologies and applications, as well as great operability. The research at home and abroad is still at a relatively preliminary stage. Therefore, it is necessary to study the effect of electrostatic force on the collision efficiency of micro-particle.

2. Force analysis of particle collision

The forces that polar particles are subjected to during a collision can be divided into two categories: internal force and external force. Internal forces mainly include van der Waals force, elastic deformation force and electrostatic force; external forces mainly include fluid drag force, capillary force and gravity. After the particle collision, the internal force is much more important than the external force. Therefore, the external force is usually ignored in the research. This paper mainly studies the internal force and adds the electrostatic force to analyze it based on the traditional research.

Van der Waals force has a weak attraction between molecules. The energy of action is generally only a few thousand to several tens of kilojoules per mole, which is one to two orders of magnitude smaller than the bond energy of a chemical bond. Its existence makes the micro-particles and the general coarse particles (particle size above 1mm) have significant differences in related kinetics and macroscopic motion laws.

When the two particles collide with each other, deformation occurs. When the particles are regarded as spheres, the two particles gradually develop into surface contact from the initial point contact.In this process, the van der Waals force of the collision between particles can be regarded as the superposition of two spheres with radius R and two planes. The expression is [10]:

$$F_{vdw} = \frac{A_{dp}}{24Z_0} + s(d_p - s) \frac{A}{6Z_0^3}$$

(1)

In the formula, $A$ is the Hamaker constant; $Z_0$ is the starting distance for the van der Waals force ($(1.65~4) \times 10^{-10}$)m; $d_p$ is the diameter of the particles; $s$ is the compression distance between the particles (calculated by the center line).

Figure 1. Inter-particle collision model
At the same time, the deformation of the particles due to the collision inevitably produces an elastic deformation force. This internal force changes continuously as the degree of particle extrusion changes. As shown in Figure 1, when one particle collides with another stationary sphere at a speed, the two particles collide and undergo deformation, and in this process, an elastic deformation force is generated. The elastic deformation force causes the two particles to produce an acceleration of opposite magnitude and opposite direction, and when the compression distance reaches a maximum, the elastic deformation force also reaches a maximum value. As shown in Figure 1, a sphere of radius R has a deformation distance of s at the moment of the collision. At this point, the geometric relationship in the figure can be expressed as:

\[ (x - (R - s))^2 + y^2 = R^2 \quad (x < 0) \]  

(2)

The expression of the elastic force is:

\[ dF_e = k_0(-x)dy \cdot 2\pi y \]  

(3)

Integrate Equation 3 to get [11]:

\[ F_e = \int dF_e = \int_{x=0}^{x=-s} \pi k_0(-x)dy = \pi k_0 \left( \frac{s^3}{3} - \frac{d_p s^2}{2} \right) \]  

(4)

Where \( k_0 \) is the stiffness of the particles, which is determined by the material of the particles. Compared with van der Waals forces and elastic deformation forces, the electrostatic forces are not of interest. The micro-particles are generally considered to be uncharged. In fact, due to the existence of friction, the general particles will carry a certain charge, even if it is a neutral particle, it will be polarized into polar particles when applied electric field.

For a finite volume of microparticles, there is an upper limit on the charge attached to it, and the microparticles do not exceed this upper limit. The upper limit of the amount of charge carried by aerosol particles and liquid particles is also different. In this paper, the aerosol particles are used for simulation. When the electric field strength and particle size are constant, the maximum amount of charge that the aerosol particles can carry is:

\[ n_m = \frac{E_s d_p^2}{4\epsilon_0} \]  

(5)

Where \( n_m \) represents the value of the maximum amount of charge that the particle can carry; \( d_p \) is the diameter of the solid particles, \( \epsilon_0 \) is the amount of charge per unit charge, and \( E_s \) is the surface electric field strength when the ionization of the particles occurs, for electronics \( E_s = 9.9 \times 10^{8} V/m \), and for ionization emissions is \( E_s = 2 \times 10^{9} V/m \). The maximum amount of charge that can be carried by a portion of the diameter particles is as described in Table 1.

| Particle diameter (nm) | Maximum charge that can be carried |
|------------------------|-----------------------------------|
| 200                    | 6.1875 \times 10^{13}             |
| 300                    | 1.3922 \times 10^{14}             |
| 400                    | 2.4750 \times 10^{14}             |
| 500                    | 3.8672 \times 10^{14}             |

As for the distribution of electric charge of the fine particles, there are two assumptions. The first one is shown in Figure 2. The charge is concentrated in the center of the particle. The calculation is simple, but there is a certain error with the actual situation. The second is shown in Figure 3. The charge is distributed on the surface of the particle and moves freely as the particle moves and collides. This assumption is closer to the actual situation than the first assumption, but the calculation is pretty complicated.
When the two particles are attracted to each other, the electrostatic force calculated according to hypothesis one will be lower than the theory, and hypothesis two will be too high. Conversely, when the two particles repel each other, the electrostatic force calculated according to hypothesis one will be higher than the theoretical value, and hypothesis two will be lower than this value. According to hypothetical one, the electrostatic force expression can be expressed as:

$$F_{\text{elec}} = \frac{1}{4\pi \varepsilon_0} \frac{q_1 q_2}{D^2}$$  \hspace{1cm} (6)

In the formula, $q_1$, $q_2$ is the amount of charge carried on the two particles, the symbol is positive when positively charged, and negative when negatively charged; $D$ is the spherical distance between two particles; $\varepsilon_0$ is the permittivity of vacuum, $\varepsilon = 8.85 \times 10^{-12} \text{F/m}$.

And the electrostatic force expression of hypothesis two can be expressed as [12, 13]:

$$F_{\text{elec}} = \frac{1}{\varepsilon D^2} \left( F_5 q_1^2 + F_6 q_1 q_2 + F_7 q_2^2 \right)$$  \hspace{1cm} (7)

Where $\varepsilon$ is the dielectric constant of the medium; $F_5, F_6, F_7$ are the complex functions related to the spherical distance $D$ and the particle diameter $d_p$.

After solving the two hypotheses, it is found that the force and energy difference calculated by the two models are small. Therefore, this paper adopts the hypothesis one model which is convenient for calculation. For the electrostatic force of particles generated by collision deformation, the expression is:

$$F_{\text{elec}} = \frac{1}{4\pi \varepsilon_0 \left( d_p - 2s \right)^2}$$  \hspace{1cm} (8)

### 3. Calculation results and discussion

#### 3.1. No electrostatic force applied

When no electrostatic force is applied, the particle collision only considers the influence of van der Waals force and elastic deformation force. When a particle collides with the other particle from the horizontal direction at a velocity of $v_0$, the equation of the particle collision can be expressed as:

$$\begin{align*}
\frac{ds}{dt} &= -v \\
\frac{dv}{dt} &= \frac{F_c - F_{\text{vdw}}}{m} \\
\left. s \right|_{t=0} &= 0 \\
\left. v \right|_{t=0} &= v_0
\end{align*}$$  \hspace{1cm} (9)
Taking the spherical spherical particles with a diameter of 300 nm as an example, solving the above differential equations, the specific parameters are shown in Table 2.

Where $k_0$ is an equation with a variable $d_p$. When $d_p = 300\text{nm}$, $k_0 = 5.4 \times 10^9$.

\[
\ln \left( \frac{k_0}{10^7} \right) = 15d_p^3 + 33d_p^2 - 29d_p + 6.3 \tag{10}
\]

| $A$ | $k_0$ | $\rho$ |
|-----|-------|--------|
| $6.8 \times 10^{-20}$ | $f(d_p)$ | $0.982 \times 10^3(kg/m^3)$ |

Using the Fourth-order Runge-Kutta method to solve the two differential equations separately, the relationship between the initial velocity $v_0$ without electrostatic force and the maximum compression distance $S_{\text{max}}$ of the particles can be obtained. Compared with the results of the previous research done by Sheng Bingying, as shown in Figure 4.

![Figure 4. $S_{\text{max}}$ and $v_0$ curves of particle collision](image)

From the figure, it can be found that the calculation results are basically consistent with the predecessors, which proves the accuracy of the data obtained in this paper.

3.2. **Electrostatic force is attractive**

When the polarities of the two particles are different, the electrostatic force causes the two particles to attract each other. At this time, the electrostatic force acts in the same direction as the van der Waals force, and the elastic deformation force acts in the opposite direction. The equations can be expressed as:

\[
\begin{cases}
\frac{ds}{dt} = -v \\
\frac{dv}{dt} = \frac{F_e - F_v + F_{\text{elec}}}{m} \\
s|t = 0 = 0 \\
v|t = 0 = v_0
\end{cases} \tag{11}
\]

Solving the two sets of differential equations by the Runge-Kutta method in MATLAB can obtain the relationship between $S_{\text{max}}$ and $v_0$ when the electrostatic force is attractive, as shown in Figure 5.
Figure 5. The relationship between $s_{\text{max}}$ and $v_0$ when electrostatic force is attractive

Figure 6. Curves of $s_{\text{max}}$ and $v_0$ when attracted to each other at different particle sizes

Comparing Figure 4 and Figure 5, it can be seen that although the trend of the relationship between $s_{\text{max}}$ and $v_0$ is substantially the same, when the electrostatic force is attractive, the magnitude of the maximum compression distance $s_{\text{max}}$ is significantly larger compared with the case where no electrostatic force is applied. Also, it can be seen from Figure 6 that the smaller the particle diameter of the particles, the larger the maximum compression distance.

This shows that when the charge polarity of the colliding particles are different, the electrostatic force causes the smaller particle size particles to close and compress each other, thereby enhancing the efficiency of particle collision and coagulation, making the particles more prone to agglomeration.

3.3. Electrostatic force is repulsion

When the polarities of the two particles are the same, the electrostatic force causes the two particles to repel each other. Now, the electrostatic force acts in the opposite direction to the Van der Waals force, when the elastic deformation force acts in the same direction. The equations can be expressed as:
Solving the two sets of differential equations by the fourth-order Runge-Kutta method in MATLAB can obtain the relationship between $S_{\max}$ and $v_0$ when the electrostatic force is attractive, as shown in Figure 7.

$$\begin{align*}
\frac{ds}{dt} &= -v \\
\frac{dv}{dt} &= \frac{F_e - F_{vdw} + F_{elec}}{m} \\
s|t = 0 &= 0 \\
v|t = 0 &= v_0
\end{align*}$$ (12)

Figure 7. The relationship between $s_{\max}$ and $v_0$ when electrostatic force is repelled

Comparing Figure 7 and Figure 4, it can be seen that the trend of the relationship between $S_{\max}$ and $v_0$ is about the same, but when the electrostatic force is repulsive, the magnitude of the maximum compression distance $S_{\max}$ is greatly reduced compared with the case where no electrostatic force is applied.

Figure 8. Curve of $S_{\max}$ and $v_0$ at different particle sizes during repulsion
Also, it can be seen from Figure 8 that when the electrostatic force is mutually exclusive, when the particle size of the particles is larger, the maximum compression distance is larger. This means that when the charge of the colliding particles is the same kind of electric charge, the electrostatic force will prevent the particles from coming close to each other, greatly reducing the compression distance when the particles collide, thereby weakening the efficiency of particle collision and coagulation, and making the particle agglomeration effect worse.

4. Conclusion

Based on the numerical simulation of the traditional particle collision process, the collision efficiency under the action of particle electrostatic force, the influence of different charge polarity types on particle collision, and the maximum charge amount of particles with different particle sizes are analyzed. Also the collision efficiency of particles under this particle size and electrostatic force are studied. It is found that when the particles have different charges, the electrostatic force attracted by each other will increase the maximum compression distance of the particle collision, thereby increasing the coagulation effect; when the particles are charged with the same kind of charge, the mutually exclusive electrostatic force reduces the maximum compression distance of the collision, thus weakening the coagulation effect. It is also found that when particles with different kinds of charges collide, the smaller the particle size, the larger the maximum compression distance, the better the coagulation effect; when the particles with the same kind of charge collide, the particles with larger particle size, the maximum compression distance is larger.

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