

An Approximate Expression for the Coagulation Coefficient of Bipolar-charged Particles in an Alternating Electric Field

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Abstract: Based on the kinetic equation of particles and the method used in Williams' research on acoustic coagulation (Aerosol Science, 1991), an approximate expression is proposed for the coagulation coefficient of bipolar-charged particles with the effect of an alternating-current (AC) electric field. When the external electric field is high enough, the proposed solution agrees well with the previous numerical results of Koizumi et al (Journal of Electrostatics, 2000).

Key words: coagulation coefficient, bipolar-charged, AC electric field

1 INTRODUCTION

The external AC electric field increases the coagulation of bipolar-charged particles effectively^{[1][2][3]}.

Zebel^[4] and Fuchs^[5] have derived the coagulation coefficient of electrically charged (including both unipolar-charged and bipolar-charged) particles by Coulomb force without the effect of any external electric fields. Wang et al.^[6] have derived the coagulation coefficient of bipolar-charged particles with the effect of an external direct-current (DC) electric field. The coagulation coefficient of bipolar-charged particles with the effect of an external AC electric field, however, is more complicated. Koizumi et al.^[7] have calculated it numerically. Here we will give an approximate expression for that, which will make the simulation of aerosol-dynamics and the computation of agglomeration equation more easily.

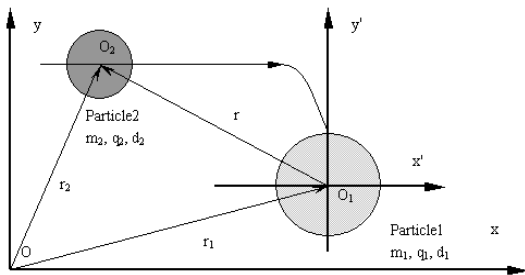


Fig. 1 The motions of two charged particles in an AC electric field. The direction of oscillation is parallel to the x-axis

2 THEORETICAL ANALYSIS

2.1 The motional Equations of Particles

Consider the coagulation between two charged particles (Fig. 1). In an AC electric field with amplitude E_0 and frequency f , the kinetic equation of a charged particle with mass m_i and charge q_i is:

$$\frac{d^2 \bar{r}_i}{dt^2} + \frac{d\bar{r}_i}{\tau_i dt} = \frac{q_i \bar{E}_0}{m_i} \cos(2\pi ft) + \frac{q_1 q_2}{4\pi \epsilon_0 m_i r^2} \frac{\bar{r}}{r}, i=1, 2 \quad (1)$$

Here \bar{r}_i is the position vector of the particle, $\bar{r} = \bar{r}_2 - \bar{r}_1$ is the relative position vector, ϵ_0 is the permittivity of free space. If the particle is spherical and Stokes drag is applicable, we have the mass as $m_i = \frac{1}{6} \rho \pi d_i^3$ and the relaxation time of the particle as $\tau_i = \frac{\rho d_i^2}{18\mu} C_{ci}$, where ρ is the particle's density, d_i is the particle's diameter, μ is the viscosity of air and C_{ci} is the Cunningham correction factor^[8]:

$$C_{ci} = 1 + \frac{1}{Pd_i} [15.60 + 7.00 \exp(-59Pd_i)] \times 10^{-3}, i=1, 2 \quad (2)$$

here P is the absolute pressure.

In the direction of oscillation (x), when the electric field is dominant (this assumption will be discussed later), the motion of the charged particle is influenced mainly by the following equation:

$$\frac{d^2 x_i}{dt^2} + \frac{dx_i}{\tau_i dt} = \frac{q_i E_0}{m_i} \cos(2\pi ft), i=1, 2 \quad (3)$$

which has the analytical solution:

$$x_i = -\frac{1}{\sqrt{1 + \tan^2 \varphi_i}} \frac{q_i E_0 C_{ci}}{6\pi^2 \mu d_i f} \sin(2\pi ft - \varphi_i), i=1, 2 + C_1 e^{-t/\tau_i} + C_2 \quad (4)$$

with the phase difference φ_i :

$$\tan \varphi_i = 2\pi f \tau_i = \frac{\pi \rho d_i^2 f}{9\mu} C_{ci}, i=1, 2 \quad (5)$$

In the following calculations, the values of the parameters are mainly taken from the study of Koizumi et al.^[7]: $E_0 < 40.0 \text{ kV/cm}$, $f = 50 \text{ Hz}$, $m = 1.8 \times 10^{-5} \text{ kg/ms}$.

The particles are charged by corona discharge in an electric field where $E_c = 2.5 \text{ kV/cm}$ and the ion density $i = 1.4 \text{ mA/m}^2$. The charge of the particles is decided by the sum of the following two charging mechanisms: the field charge q_f and the diffusion charge q_d :

$$q_f = \frac{3\pi\epsilon_0\epsilon_r d^2}{\epsilon_r + 2} E_c \frac{t/\tau_f}{1 + t/\tau_f}, \quad (6)$$

$$q_d = \frac{2\pi d \epsilon_0 \kappa T}{e} \ln\left(1 + \frac{t}{\tau_d}\right) \quad (7)$$

where ϵ_r is the particle's relative dielectric constant, e is the unit charge, κ is the Boltzmann constant, T is the absolute temperature, τ_f and τ_d are the time constants for field charging and diffusion charging, respectively. Then φ_i and the second term on the right-hand side of Eq. (4) can be ignored, and there is a very good approximation of solution (4) for the particles with diameter $d_i < 20 \text{ mm}$:

$$x_i = -X_i \sin(2\pi f t), \quad i=1, 2 \quad (8)$$

where the oscillation amplitude is:

$$X_i = \frac{q_i E_0 C_{ci}}{6\pi^2 \mu d_i f}, \quad i=1, 2 \quad (9)$$

And the velocity amplitude of the particle will be:

$$V_i = 2\pi f \cdot X_i = \frac{q_i E_0 C_{ci}}{3\pi \mu d_i}, \quad i=1, 2 \quad (10)$$

In the y direction, there is no external electric field. The kinetic equation of the particle is:

$$\frac{d^2 y_i}{dt^2} + \frac{dy_i}{\tau_i dt} = \frac{q_1 q_2}{4\pi \epsilon_0 m_i r^2} \frac{y_i}{r}, \quad i=1, 2 \quad (11)$$

Because of the difficulty of solving Eq. (11), we here treat it in a special case where $X_i = 0$ and $\frac{d^2 y_i}{dt^2} = 0$. Then we set $y = y_2 - y_1$ and get:

$$\frac{dy}{dt} = \frac{q_1 q_2}{4\pi \epsilon_0 y^2} \frac{\tau_1}{m_1} + \frac{\tau_2}{m_2} \frac{\ddot{y}}{\ddot{y}} \quad (12)$$

which has the analytical solution:

$$y = \sqrt[3]{\frac{3q_1 q_2}{4\pi \epsilon_0} \left(\frac{\tau_1}{m_1} + \frac{\tau_2}{m_2} \right) t} + C_3 \quad (13)$$

Now we assume that the solution of Eq. (11) has a similar form to that of Eq. (12). Then the distance in the y direction between the two particles can be written as:

$$Y = \sqrt[3]{C_4 \frac{3q_1 q_2}{4\pi \epsilon_0} \left(\frac{\tau_1}{m_1} + \frac{\tau_2}{m_2} \right) \frac{y_0}{X} t} \quad (14)$$

Here C_4 is a constant, $y_0/X = \cos(\alpha_0)$, where $\angle \alpha_0$ is taken as an approximate average of $\angle O_2 O_1 y'$ (refer to Fig. 1) during the period of oscillation, and $X = X_1 + X_2$ because of the opposite charge of the two particles.

Furthermore, by setting constant $C_5 = C_4 y_0$ and using

$$\tau_i = \frac{r d_i^2}{18m} C_{ci}, \quad m_i = \frac{1}{6} r \pi d_i^3, \quad \text{solution (14) becomes:}$$

$$Y = \sqrt[3]{C_5 \frac{q_1 q_2}{4\pi^2 \mu \epsilon_0 (X_1 + X_2)} \left(\frac{C_{c1}}{d_1} + \frac{C_{c2}}{d_2} \right) t} \quad (15)$$

In this article, y_0 is in the order of $d_i (\approx 10^{-6})$, and C_4 is in the order of $d_i/X_i (\approx 10^{-2})$. According to the numerical calculation, we at last get $C_5 \approx 0.5 \times 10^{-8}$.

2.2 The Coagulation Coefficient of Particles

The coagulation coefficient can be defined as the effective particles collision volume per second and the unit of which is m^3/s . When an external electric field exists, it can be approximately expressed as $K_e = S \cdot V$, where S is the collision cross section and V is the relative velocities between the particles.

Wang et al.^[6] have given the coagulation coefficient of bipolar-charged particles in an external DC electric field:

$$K_{ej-DC} = \frac{q_1 q_2 (d_1 + d_2)}{3\pi \epsilon_0 \mu d_1 d_2} + \frac{(d_1 + d_2)^2}{12\mu} E_0 \left(\frac{q_1}{d_1} C_{c1} + \frac{q_2}{d_2} C_{c2} \right) \quad (16)$$

The first term on the right-hand side of Eq. (16) is based on the coagulation coefficient of bipolar-charged particles by Coulomb force without the effect of an external electric field, which is given by Zebel^[4] and Fuchs^[5]. The second term about the external force is derived by using the method of Williams et al.^[9]:

$$K_e = S \cdot V = \frac{1}{4} \pi (d_1 + d_2)^2 \cdot |v_1 - v_2| \quad (17)$$

The terms are applicable in the continuum regime where the Knudsen number of a particle is small.

Now when we consider the coagulation coefficient of bipolar-charged particles in an AC electric field, we can use Eq. (17) and the first term on the right-hand side of Eq. (16) in the same way.

Because the particles attract each other by Coulomb force when they approach during the oscillation, the external AC electric field has an additional effect on the collision cross section:

$$S = \frac{\pi}{4} (d_1 + d_2 + 2Y_{AC})^2 \quad (18)$$

where Y_{AC} is assumed to be decided by Eq. (15) with the time $t = 1 \text{ s}$:

$$Y_{AC} = \sqrt[3]{C_5 \frac{q_1 q_2}{4\pi^2 \mu \epsilon_0 (X_1 + X_2)} \left(\frac{C_{c1}}{d_1} + \frac{C_{c2}}{d_2} \right)} \quad (19)$$

The relative velocity between the two particles can be assumed as the difference between the two average velocities in the oscillation direction:

$$V = \frac{2}{\pi} |V_1 - V_2| = \frac{2}{3\pi^2 \mu} E_0 \left(\frac{q_1}{d_1} C_{c1} + \frac{q_2}{d_2} C_{c2} \right) \quad (20)$$

Then referring to Eq. (16) and combining Eq. (18) and (20), we get the coagulation coefficient of bipolar-charged particles in an AC electric field:

$$K_{ej-AC} = \frac{q_1 q_2 (d_1 + d_2)}{3\pi \epsilon_0 \mu d_1 d_2} + \frac{(d_1 + d_2 + 2Y_{AC})^2}{6\pi \mu} E_0 \left(\frac{q_1}{d_1} C_{c1} + \frac{q_2}{d_2} C_{c2} \right) \quad (21)$$

3 RESULTS AND DISCUSSIONS

Here the approximate expression for the coagulation coefficient of bipolar-charged particles with the effect of an external AC electric field is estimated and discussed. In order to validate the expression (21), we compare it with the previous numerical results of Koizumi et al.^[7]

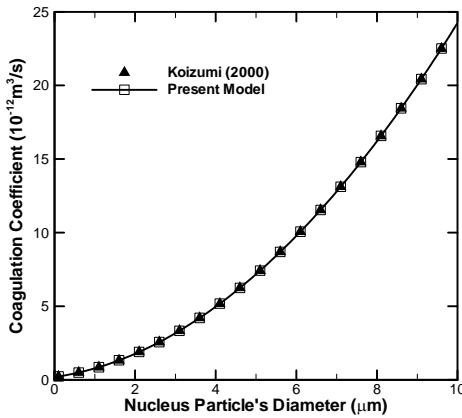


Fig. 2 Coagulation coefficient of bipolar-charged particles by Coulomb force without the effect of any external electric field

First let us consider the case without any external electric field ($E_0 = 0$). Wang et al.^[6] have proved that in this situation the coagulation coefficient can be reduced to the solution of Zebel^[4] and Fuchs^[5]. Fig. 2 shows the results. Both particles are assumed to be solid carbon whose relative dielectric constant ϵ_r is 3. One particle's diameter is 1 nm, and the other's varies from 0.1 nm to 10.0 nm.

Then here comes the case with an external AC electric field. The coagulation coefficients are shown in Fig. 3 and Fig. 4. Note that the abscissa value of E_0 is not a RMS, but the amplitude of the AC electric field. The results are compared with the numerical simulation of Koizumi et al.^[7]

Fig. 5 and Fig. 6 give the estimates of the errors between the approximate expression and the numerical results. Because the effect of Coulomb force becomes stronger when the particles are closer, this approximation works better with higher electric field, which makes the particles' amplitude larger. For the coagulation coefficient of carbon particles with a diameter of 1 nm, the estimates of errors will be less than 3.0% when the external electric field is over 15.0 kV/cm. For the coagulation coefficient of particles of 1 nm and 10 nm,

the estimates of errors will be less than 3.0% when the external electric field is over 3.0 kV/cm.

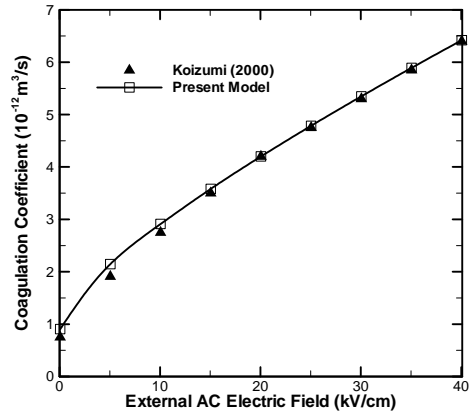


Fig. 3 Coagulation coefficient of bipolar-charged particles with the effect of an external AC electric field. Both carbon particles have a diameter of 1 nm

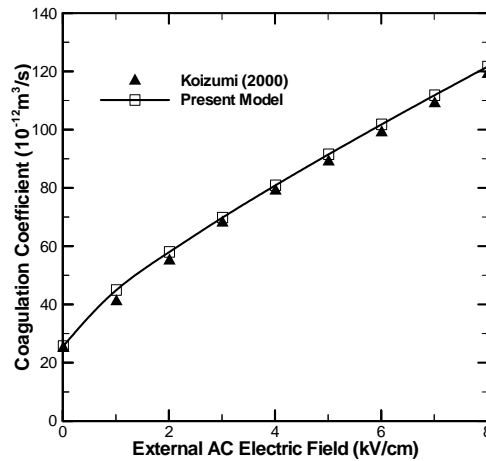


Fig. 4 Coagulation coefficient of bipolar-charged particles with the effect of an external AC electric field. One particle has a diameter of 1 nm; the other has a diameter of 10 nm

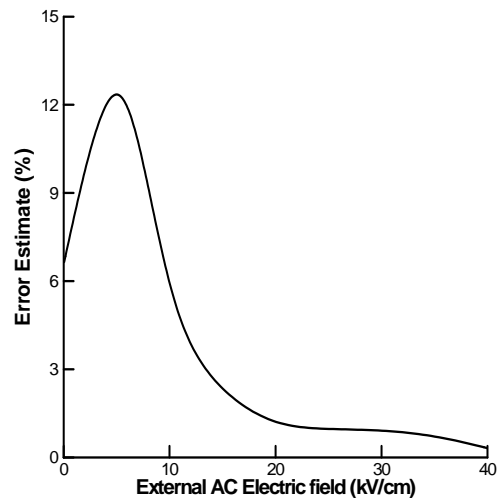


Fig. 5 Error estimate between the approximate expression and the numerical results. Both carbon particles have a diameter of 1 nm

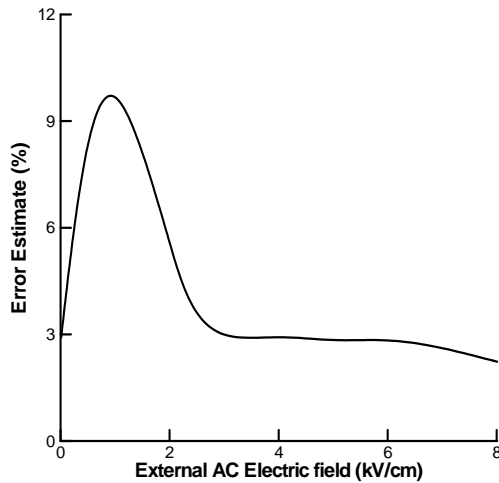


Fig. 6 Error estimate between the approximate expression and the numerical results. One particle has a diameter of 1 nm ; the other has a diameter of 10 nm

When we derive Eq. (3), we assume that the electric field is dominant. Now consider the ratio of the electric force to the Coulomb force in the direction of x-axis:

$$R = \frac{4\pi\epsilon_0 r^2 E_0 \cos(2\pi ft)}{q_j \sin \alpha}, \quad j=1, 2 \quad (22)$$

where $\angle \alpha = \angle O_2 O_1 y'$ (refer to Fig. 1).

Approximately, the charge of the particle can be get from Eq. (6) and $\sin \alpha$ changes in step with $\cos(2\pi ft)$. Then Eq. (22) can be written as:

$$R = \frac{4(\epsilon_r + 2)r^2 E_0}{3\epsilon_r d_j^2 E_c}, \quad j=1, 2 \quad (23)$$

Because the minimum of r equals $0.5(d_1 + d_2)$, the ratio R will be more than 1.0 in most places when the electric field E_0 is large enough, for example, larger than E_c .

Compared with the effect of an external DC electric field, the AC electric field causes a bigger collision cross section S and a smaller relative velocity V . But as a whole, the AC electric field is more effective for particles' coagulation than DC.

The expression for the coagulation coefficient of bipolar-charged particles in an AC electric field is based on the kinetic equation of particles and the Stokes collision model, which both assume the Stokes law is applicable. So the Reynolds number Re_D should be small enough, which means neither the particle's diameter nor the electric field can be too large.

Finally, the present approximate model is based on the collision between two charged particles. The actual coagulation of bipolar-charged particles should involve the

interactions of a lot of particles and would be more complicated.

4 CONCLUSIONS

Based on the kinetic equation of particles and the method used in Williams' research on acoustic coagulation^[9], an approximate expression for the coagulation coefficient of bipolar-charged particles with the effect of an external AC electric field is proposed. This expression is compared with the numerical results of Koizumi et al.^[7]. For the carbon particles with a diameter of 1 nm, the error estimates between the expression and the numerical results will be less than 1.0% when the external electric field is over 20.0 kV/cm. For the carbon particles of 1 nm and 10 nm, the estimates of errors will be less than 3.0% when the external electric field is over 3.0 kV/cm.

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