ELECTROSTATIC BARRIER AGAINST DUST GROWTH IN PROTOPLANETARY DISKS. I. CLASSIFYING THE EVOLUTION OF SIZE DISTRIBUTION

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ABSTRACT

Collisional growth of submicron-sized dust grains into macroscopic aggregates is the first step of planet formation in protoplanetary disks. These grains are expected to carry nonzero negative charges in the weakly ionized disks, but its effect on their collisional growth has not been fully understood so far. In this paper, we investigate how the charging affects the evolution of the dust size distribution properly taking into account the charging mechanism in a weakly ionized gas as well as porosity evolution through low-energy collisions. To clarify the role of the size distribution, we divide our analysis into two steps. First, we analyze the collisional growth of charged aggregates assuming a monodisperse (i.e., narrow) size distribution. We show that the monodisperse growth stalls due to the electrostatic repulsion when a certain condition is met, as was already expected in our previous work. Second, we numerically simulate dust coagulation using Smoluchowski’s method to see how the outcome changes when the size distribution is allowed to freely evolve. We find that, under certain conditions, the dust undergoes bimodal growth where only a limited number of aggregates continue to grow, carrying a major part of the dust mass in the system. This occurs because remaining small aggregates efficiently sweep up free electrons to prevent the larger aggregates from being strongly charged. We obtain a set of simple criteria that allows us to predict how the size distribution evolves for a given condition. In Paper II, we apply these criteria to dust growth in protoplanetary disks.

Key words: dust, extinction – planets and satellites: formation – protoplanetary disks

1. INTRODUCTION

The standard core-accretion scenario for planet formation (Mizuno 1980; Pollack et al. 1996) is based on the so-called planetesimal hypothesis. This hypothesis assumes that solid bodies of size larger than kilometers (called “planetesimals”) form in a protoplanetary disk prior to planet formation. However, the typical size of solid particles in interstellar space is as small as a micron or even smaller (Mathis et al. 1977). How the submicron-sized grains evolved into kilometer-sized planetesimals is not yet fully understood.

The simplest picture for dust evolution toward planetesimals can be summarized into the following steps. (1) Initially, submicron-sized particles coagulate into larger but highly porous, fractal aggregates through low-velocity collisions driven by Brownian motion and differential settling toward the midplane of the disk (Wurm & Blum 1998; Blum et al. 1998; Kempf et al. 1999). (2) As the aggregates grow to “macroscopic” (millimeter to centimeter) sizes, the collisional energy becomes high enough to cause the compaction of the aggregates (Blum 2004; Suyama et al. 2008; Paszun & Dominik 2009). (3) The compaction causes an increase in the stopping times of the aggregates, allowing them to concentrate in the midplane of the disk (Safronov 1969; Goldreich & Ward 1973), the center of vortices (Barge & Sommeria 1995), or turbulent eddies (Johansen et al. 2007). (4) Planetesimals may form within such dense regions through gravitational instability (Safronov 1969; Goldreich & Ward 1973) or through further collisional growth (Weidenschilling & Cuzzi 1993; Weidenschilling 1995).

However, there is great uncertainty on how large dust aggregates can grow through mutual collisions (see, e.g., Blum & Wurm 2008; Gütter et al. 2010). As the collisional compaction proceeds, the aggregates decouple from the ambient gas and obtain higher and higher relative velocities driven by radial drift (Weidenschilling 1977) and gas turbulence (Völk et al. 1980). The collision velocity can exceed 10 m s⁻¹ even without turbulence, but it is uncertain whether such high-speed collisions lead to the sticking or fragmentation of the aggregates (Blum & Wurm 2008; Wada et al. 2009; Teiser & Wurm 2009; Gütter et al. 2010). In addition, collisional compaction itself can cause the reduction of sticking efficiency (Blum & Wurm 2008; Gütter et al. 2010). This may terminate the collisional growth before the fragmentation occurs (Zsom et al. 2010).

By contrast, it is generally believed that dust coagulation proceeds rapidly until the aggregates grow beyond the initial, fractal growth stage since the collision velocity is too low to cause the reduction of sticking efficiency (Dominik & Tielens 1997; Blum & Wurm 2008; Gütter et al. 2010). However, one of the authors has recently pointed out that electric charging of aggregates could halt dust growth before the aggregates leave this stage (Okuzumi 2009, hereafter O09). Protoplanetary disks are expected to be weakly ionized by various kinds of high-energy sources, such as cosmic rays (Umebayashi & Nakano 1981) and X-rays from the central star (Glassgold et al. 1997). In such an ionized environment, dust particles charge up by capturing ions and electrons, as is well known in plasma physics (Shukla & Mamun 2002). In equilibrium, dust particles acquire nonzero negative net charges because electrons have higher thermal velocities than ions. This “asymmetric” charging causes a repulsive force between colliding aggregates, but this effect has been ignored in previous studies on protoplanetary dust growth. O09 has found that the dust charge in a weakly ionized disk can be considerably smaller than in a fully ionized plasma but can nevertheless inhibit dust coagulation in a wide region of the disk. It is also found that the electrostatic barrier becomes significant when the dust grows into fractal aggregates.
much earlier than the growth barriers mentioned above emerge. Thus, the dust charging can greatly modify the current picture of dust evolution toward planetesimals.

The analysis of the electrostatic barrier by O09 is based on the assumption that dust aggregates obey a narrow size distribution. In reality, however, the size distribution is determined as a result of the coagulation process, and it has been unclear how the distribution evolves when dust charging is present. The purpose of this study is to clarify how the size distribution of dust aggregates evolves when the aggregates are charged in a weakly ionized gas.

According to O09, the effect of dust charging can become significant before the collisional compaction of aggregates becomes effective. In this stage, dust aggregates are expected to have increasingly lower internal density (i.e., increasingly higher porosity) as they grow, as suggested by laboratory experiments and $N$-body simulations (Wurm & Blum 1998; Blum et al. 1998; Kempf et al. 1999). This porosity evolution has been ignored in most theoretical studies on dust coagulation (e.g., Nakagawa et al. 1981; Tanaka et al. 2005; Brauer et al. 2008), in which aggregates are simplified as compact spheres. However, when analyzing the electrostatic barrier, the porosity evolution must be accurately taken into account; in fact, as we will see later, the ignorance of the porosity evolution leads to considerable underestimation of the electrostatic barrier, because compact spheres are generally less coupled to the ambient gas and hence have higher collision energies than porous aggregates. In this study, we use the fractal dust model recently proposed by Okuzumi et al. (2009, hereafter OTS09). Classically, fractal dust growth has been modeled only with either of its two extreme limits, namely, ballistic cluster–cluster and particle–cluster aggregation (BCCA and BPCA; e.g., Ossenkopf 1993; Dullemond & Dominik 2005). To fill the gap between the two limits, OTS09 introduced a new aggregation model (called the quasi-BCCA model) in which aggregates grow through unequal-sized collisions. OTS09 found from $N$-body simulations that the resultant aggregates tend to have a fractal dimension $D$ close to 2 even if the size ratio deviates from unity. This explains why fractal aggregates with $D \sim 2$ are universally observed in various low-velocity coagulation processes (Wurm & Blum 1998; Blum et al. 1998; Kempf et al. 1999). OTS09 summarized the results of their $N$-body simulations into a simple analytic formula giving the increase in the porosity (volume) for general hit-and-stick collisions. This formula together with the Smoluchowski equation extended for porous dust coagulation (OTS09) enables us to follow the evolution of the size distribution and porosity consistently with dust charging.

As we will see later, our problem involves many model parameters, such as the initial grain size and the gas ionization rate. To fully understand the dependence of the results on these parameters, we do not assume any protoplanetary disk model but seek to find general criteria determining the outcome of dust evolution. This approach allows us to investigate the effect of the electrostatic barrier with any protoplanetary disk models. Application of the growth criteria to particular disk models is addressed in Paper II (Okuzumi et al. 2011).

This paper is structured as follows. In Section 2, we describe the dust growth model considered in this study. We consider collisional growth of dust starting from an ensemble of equal-sized spherical grains (“monomers”). Each aggregate is characterized by its mass, radius, projected area, and charge. For simplicity, we assume “local” growth, i.e., we neglect global transport of dust within a disk.

We focus on the first stage of dust evolution in protoplanetary disks and assume that aggregates grow through “hit-and-stick” collisions, i.e., collisions with perfect sticking efficiency and no compaction. It is known theoretically (e.g., Kempf et al. 1999) and experimentally (e.g., Wurm & Blum 1998) that hit-and-stick collisions lead to highly porous aggregates. To take into account the porosity evolution, we adopt the fractal dust model proposed by OTS09. This model characterizes each aggregate with its mass $M$ and “characteristic radius” $a$ (see OTS09 and Section 2.3 for the definition of the characteristic radius), and treat the two quantities as independent parameters. Another important parameter is the projected area $A$. This determines how the aggregates are fractionally coupled to the gas. In the OTS09 model, $A$ is not treated as an independent parameter but is given as a function of $M$ and $a$. Note that $A$ is not generally equal to a naive “cross section” $\pi a^2$, especially when the aggregates are highly porous (Figure 1; see also Figure 4 of OTS09).

Distinction between $A$ and $\pi a^2$ allows us to avoid overestimation of the gas drag force to dust aggregates. In Section 2.3, we will describe the porosity model in more detail.

Figure 1. Projection of a numerically created, three-dimensional porous aggregate consisting of $\approx 1000$ monomers. The large open circle shows the characteristic radius $a$ (for its definition, see Section 2.3.1), while the gray disk inside the circle shows the projected area $A$ averaged over various projection angles. Note that $A$ is not necessarily equal to $\pi a^2$, especially when the aggregate is highly porous (see also Figure 4 of OTS09).

2. DUST GROWTH MODEL

In this section, we describe the dust growth model considered in this study.

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The collision probability for two aggregates 1 and 2 with charges \( Q_1 \) and \( Q_2 \) is proportional to their relative speed \( \Delta u \) times the collisional cross section \( \sigma_{\text{coll}} \) given by (e.g., Landau & Lifshitz 1976)

\[
\sigma_{\text{coll}} = \begin{cases} 
\pi(a_1 + a_2)^2 \left(1 - \frac{E_{\text{kin}}}{E_{\text{kin}}}ight), & E_{\text{kin}} > E_{\text{el}} \\
0, & E_{\text{kin}} \leq E_{\text{el}},
\end{cases}
\]  

where \( E_{\text{kin}} = M \mu_\text{a}(\Delta u)^2/2 \) is the kinetic energy associated with the relative motion, \( M = M_1 M_2/(M_1 + M_2) \) is the reduced mass, and \( E_{\text{el}} = Q_1 Q_2/(a_1 + a_2) \) is the energy needed for the aggregates to collide with each other. In this paper, \( E_{\text{el}} \) is called “the electrostatic energy” for colliding aggregates. Below, we describe how to determine \( Q \) and \( \Delta u \).

### 2.1. Charging

We adopt the dust charging model developed by O09. In this model, dust aggregates are surrounded by a weakly ionized gas and charged up by capturing free electrons and ions. These ionized particles are created by the nonthermal ionization of the neutral gas and are removed from the gas phase through the adsorption to the dust as well as the gas-phase recombination. The dust charge \( Q \) and the number densities of ions and electrons are thus determined by the balance among the ionization, recombination, and dust charging. In equilibrium, the average charge \( \langle Q \rangle_a \) of aggregates with radius \( a \) is given by (see Equation (23) of O09)

\[
\langle Q \rangle_a = -\Psi \frac{ak_B T}{e},
\]  

where \( k_B \) is the Boltzmann constant, \( T \) is the gas temperature, \( e \) is the elementary charge, and \( \Psi \) is a dimensionless quantity characterizing the charge state of the gas–dust mixture. O09 has analytically shown that the equilibrium conditions are reduced to a single equation for \( \Psi \). When the adsorption to the dust dominates the removal of the ionized gas, the equation for \( \Psi \) is written as (see Equation (34) of O09)

\[
\frac{1}{1 + \Psi} = \frac{s_i}{s_e} \sqrt{\frac{m_i}{m_e}} \exp \Psi - \frac{\Theta}{\Theta} = 0,
\]  

where \( m_{i(e)} \) is the mass of ions (electrons), \( s_{i(e)} \) is their sticking probability onto a dust monomer, and

\[
\Theta = \frac{\zeta n_e e^2}{s_i A_{\text{tot}} C_{\text{tot}} k_B T} \sqrt{\frac{\pi m_i}{8 k_B T}}
\]  

is a dimensionless quantity depending on the total projected area \( A_{\text{tot}} = \int A(M)n(M)dM \) and total radius \( C_{\text{tot}} = \int \alpha(M) n(M) dM \) of aggregates, and the ionization rate \( \zeta \) and number density \( n_e \) of neutral gas particles. Equation (3) originates from the quasi-neutrality condition, \( en_i = en_e + Q_{\text{tot}} = 0 \), where \( n_i \) and \( n_e \) are the number densities of ions and electrons, respectively, and \( Q_{\text{tot}} = \int \langle Q \rangle_a n(M) n(M) dM \) is the total charge carried by dust in a unit volume.\(^5\) Equation (3) cannot be used when the gas-phase recombination dominates the removal

\(^5\) \( n_i \) and \( n_e \) are related to \( \Psi \) as (O09)

\[
n_i = \frac{\zeta n_e}{s_i A_{\text{tot}} k_B T} \sqrt{\frac{\pi m_i}{8 k_B T}} \frac{1}{1 + \Psi}, \quad n_e = \frac{\zeta n_e}{s_e A_{\text{tot}} k_B T} \sqrt{\frac{\pi m_e}{8 k_B T}} \exp \Psi.
\]  

Figure 2. Schematic illustration of an ion–electron plasma (IEP: left) and an ion–dust plasma (IDP: right). In an IEP, the dominant carriers of negative charges are free electrons. In an IDP, by contrast, the dominant negative species is the charged dust. The absolute value of the dust surface potential, \( |\psi| = a|Q| \), is generally smaller in IDPs than in IEPs.

In typical protoplanetary disks, however, the gas-phase recombination can be safely neglected unless the dust-to-gas mass ratio is many orders of magnitude smaller than interstellar values \( \sim 0.01 \) (O09).

Physically, \( \Psi \) is related to the surface potential of aggregates. For an aggregate with charge \( Q \) and radius \( a \), the surface potential \( \psi \) is given by \( \psi = Q/a \). Equation (2) implies that \( \Psi = \langle \psi \rangle_a/(e k_B T) \), namely, \( \Psi \) is the surface potential averaged over aggregates of radius \( a \) and normalized by \( -k_B T/e \). Note that \( \langle \psi \rangle_a \) is apparently independent of \( a \), but actually is not because \( \Psi \) depends on the size distribution of aggregates through \( A_{\text{tot}} \) and \( C_{\text{tot}} \). It should also be noted that the radius \( a \) can be interpreted as the electric capacitance \( C \) (i.e., \( Q = C \psi \)). This is the reason why we have denoted the total radius as \( C_{\text{tot}} \).

As shown in O09, \( \Psi \) asymptotically behaves as (see Section 2.3 of O09)

\[
\Psi \approx \left\{ \begin{array}{ll}
\Psi_\infty & \text{if } \Theta \gg \Psi_\infty, \\
\Theta & \text{otherwise},
\end{array} \right.
\]  

where \( \Psi_\infty \) is the solution to

\[
\frac{1}{1 + \Psi_\infty} = \frac{s_i}{s_e} \sqrt{\frac{m_i}{m_e}} \exp \Psi_\infty = 0.
\]  

Equation (6) is known as the equation for the equilibrium charge of a dust particle embedded in a fully ionized plasma (Spitzer 1941; Shukla & Mamun 2002). Equation (5) suggests that the charge state of dust particles in a weakly ionized gas is characterized by two limiting cases. If \( \Theta \gg \Psi_\infty \), the total negative charge \( |Q|_\text{tot} \) carried by dust aggregates is negligibly small compared with \( en_e \), and the quasi-neutrality condition approximately holds in the gas phase, i.e., \( n_i \approx n_e \). If \( \Theta \ll \Psi_\infty \), by contrast, most of the negative charge in the system is carried by aggregates, and the quasi-neutrality condition approximately holds between ions and negatively charged dust. For this reason, O09 referred to the former phase as the ion–electron plasma (IEP), and to the latter as the ion–dust plasma (IDP). Figure 2 schematically shows the difference between the two plasma states.

For given \( m_i \) and \( s_i/s_e \), Equation (3) determines \( \Psi \) as a function of \( \Theta \). In typical protoplanetary disks, the dominant ion species are molecular ions (e.g., HCO\(^+\)) or metal ions (e.g., Mg\(^+\)) depending on the abundance of metal atoms in the gas phase (Sano et al. 2000; Ilgner & Nelson 2006). Although \( s_i \) is likely to be close to unity (Umeyashii & Nakano 1980; Draine...
The ion mass is taken to be 24. This is not true for more general cases. In fact, Equations (3) and (6) can be combined into a single equation (Equation (33)), which cannot be reduced to an equation for $\Psi/\Psi_{\infty}$ depending only on $\Theta/\Psi_{\infty}$.

where $\Delta u_D$ is the difference of the drift velocities between the two aggregates. Here, we have assumed that the systematic motion has no fluctuating component, that is, the velocity dispersion is thermal even when $M_u(\Delta u_D)^2 \gg k_B T$. We will discuss the effect of adopting a different velocity distribution in Section 5.3.

We further assume that aggregates are fractionally coupled to the ambient gas, and give $\Delta u_D$ as

$$\Delta u_D = g(\tau_1 - \tau_2),$$

where $\tau_j (j = 1, 2)$ is the stopping time of each aggregate and $g$ is the uniform acceleration. In this study, we focus on small aggregates and give $\tau$ according to Epstein’s law,

$$\tau = \frac{3M}{4\rho_g A} \sqrt{\frac{\pi m_g}{8k_B T}},$$

where $\rho_g$ is the gas density and $m_g$ is the mass of the gas particles.

In a protoplanetary disk, relative motion like Equation (9) is driven by several processes. For example, the gravity of the central star causes acceleration $g = \Omega_k z$ toward the midplane of the disk, where $\Omega_k$ is the Kepler rotational frequency and $z$ is the distance from the midplane. Another example is the acceleration driven by gas turbulence in the strong coupling limit. When both of two colliding aggregates are fractionally well coupled to the turbulent eddies of all scales, the relative velocity between the aggregates is approximately given by $\Delta u_D \approx (u_{\eta}/t_{\eta})(t_1 - t_2)$, where $u_{\eta}$ and $t_{\eta}$ are the characteristic velocity and turnover time for the smallest eddies, respectively (Weidenschilling 1984; Ormel & Cuzzi 2007). This means that turbulence behaves as an effective acceleration field of $g \approx u_{\eta}/t_{\eta}$ for strongly coupled aggregates.

As the collisional cross section $\sigma_{\text{coll}}$ depends on the stochastic variable $\Delta u$, it is useful to treat collision events statistically. To do so, we introduce the collisional rate coefficient

$$K \equiv \int P_1(\Delta u) |\Delta u| d\Delta u.$$

With Equations (1) and (8), the integration can be analytically performed. Using $Q_1, Q_2 > 0$, we have (Shull 1978)

$$K = \pi(a_1 + a_2)^2 \frac{k_B T}{2\pi M_u E_D} \left[ {y_+ \exp(-y_+^2) - y_- \exp(-y_-^2)} \right] + \frac{\sqrt{\pi}}{2} (1 - 2y_+ y_-) \left[ \text{erf}(y_+) - \text{erf}(y_-) \right],$$

where $\text{erf}(y) = (2/\sqrt{\pi}) \int_0^y \exp(-z^2) dz$ is the error function, and $y_+$ and $y_-$ are defined as

$$y_{\pm} = \frac{\sqrt{\Delta E}}{\pm \sqrt{E_D}}.$$

with

$$E_D = \frac{M_u(\Delta u_D)^2}{2k_B T},$$

$$E_\Delta = \frac{Q_1 Q_2}{(a_1 + a_2) k_B T}.$$

Note that $E_D$ and $E_\Delta$ are the relative kinetic energy associated with differential drift and the electrostatic energy normalized by $k_B T$, respectively.

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**Figure 3.** Comparison between the numerical solutions to Equation (3) and the approximate formula (7). The symbols indicate the numerical solutions for various values of $\Psi_{\infty}$, and the solid curves show the prediction from Equation (7). The ion mass is taken to be 24$m_u$ for all the cases. The maximum values $\Psi_{\infty}$ are 3.78, 2.81, 1.96, and 1.10 for $\Psi_{\infty}$ = 1.0, 0.3, 0.1, and 0.03, respectively.

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This is not true for more general cases. In fact, Equations (3) and (6) can be combined into a single equation (Equation (33)), which cannot be reduced to an equation for $\Psi/\Psi_{\infty}$ depending only on $\Theta/\Psi_{\infty}$.
Equation (12) has the following simple asymptotic forms:

$$K \approx \frac{\pi (a_1 + a_2)^2 \Delta u_B \exp(-\xi E)}{\pi (a_1 + a_2)^2 \Delta u_D \left(1 - \frac{\xi E}{\xi E_0}\right)}, \quad \xi E \ll 1, \quad \xi E_0 \gg 1, \quad \xi E$$

where $\Delta u_B = (8k_B T / \pi M_p)^{1/2}$ is the mean thermal speed between the colliding aggregates. The exponential factor $\exp(-\xi E)$ originates from the high-energy tail of the Maxwell distribution. This factor guarantees that $K$ is nonvanishing even for large $\xi E$.

### 2.3. Porosity Model

As shown by O09, the charging affects dust growth before the collisional compaction becomes effective. In this early stage, aggregates have a highly porous structure (Wurm & Blum 1998; Kempf et al. 1999). The porosity influences their collisional growth through the collisional and aerodynamical cross sections. It also affects dust charging through the capacity ($=\text{radius}$) and the capture cross section for ions and electrons. Therefore, it is important to adopt a realistic model for the porosity of aggregates.

In this study, we adopt the porosity model developed by OTS09. This model is based on $N$-body simulations of successive collisions between aggregates of various sizes. This model provides a natural extension of the classical hit-and-stick aggregation models (see OTS09, and references therein). Collisional fragmentation and restructuring is not taken into account, so the porosity increase only depends on the physical sizes of colliding aggregates. This assumption is valid as long as the collisional energy is sufficiently lower than the critical energy for the onset of collisional compaction. The validity of this assumption will be discussed in Section 5.4.

#### 2.3.1. Porosity Increase After Collision

Our porosity model measures the size of a porous aggregate with the characteristic radius $a \equiv [(5/3)N \sum_{k=1}^{N} (x_k - X)^2]^{1/2}$, where $N$ is the number of constituent monomers within the aggregate, $x_k$ is the coordinate of the $k$th constituent monomer, and $X$ is the center of mass. Figure 1 shows the characteristic radius as well as the projected area $A$ of a numerically created porous aggregate. In our model, the porosity of each aggregate is characterized by $a$ and $N$, while the projected area $A$ is assumed to be a function of them. In the following subsections, we summarize how $a$ and $N$ are calculated in this model.

The porosity evolution of aggregates after a collision is expressed in terms of the increase in the porous volume $V \equiv (4\pi/3) a^3$. For a collision between aggregates with volumes $V_1$ and $V_2 (\leq V_1)$, the volume of the resulting aggregate, $V_{1+2}$, can be generally written as

$$V_{1+2} = V_1 + (1 + \chi) V_2,$$

where $\chi$ is a dimensionless factor depending on $V_1$ and $V_2$. We refer to $\chi$ as the “void factor” since it definitely vanishes for compact aggregation.

It is known that there are two limiting cases for hit-and-stick collisions (see, e.g., Mukai et al. 1992; Kozasa et al. 1993). One is called BCCA, where aggregates grow only through equal-sized collisions. On average, the characteristic radius of BCCA clusters is related to the monomer number $N$ as

$$a_{\text{BCCA}} \approx a_0 N^{1/D_{\text{BCCA}}},$$

where $a_0$ is the radius of monomers and $D_{\text{BCCA}} \approx 1.9$ is the fractal dimension of BCCA clusters (e.g., Mukai et al. 1992).

The void factor for BCCA growth can be calculated from Equation (18) as $\chi_{\text{BCCA}} = 2^{3/D_{\text{BCCA}}} - 2 \approx 0.99$ (OTS09). The opposite limit is called BPCA, in which an aggregate grows by colliding with monomers. On average, the characteristic radius of BPCA clusters is given by $a_{\text{BPCA}} \approx (1 - P_{\text{BPCA}})^{-1/3} a_0 N^{1/3}$, where $P_{\text{BPCA}} \approx 0.874$ is the porosity of BPCA clusters (e.g., Kozasa et al. 1993). The void factor is found to be $\chi_{\text{BPCA}} = P_{\text{BPCA}}/(1 - P_{\text{BPCA}}) \approx 6.94$ (OTS09). Note that both $\chi_{\text{BCCA}}$ and $\chi_{\text{BPCA}}$ are constant.

To obtain $\chi$ for more general cases, OTS09 presented a new aggregation model called “quasi-BCCA” (QBCCA). In the QBCCA model, an aggregate grows through unequal-sized collisions with a fixed mass ratio $N_2/N_1$, where $N_1$ and $N_2(<N_1)$ are the monomer numbers of the target and projectile, respectively. The projectile is chosen among the outcomes of earlier collisions, so that the resultant aggregate has a self-similar structure. OTS09 performed $N$-body simulations of aggregate collisions with various size ratios and found that the void factor for QBCCA is approximately given by

$$\chi_{\text{QBCCA}}(V_1/V_2) = \chi_{\text{BCCA}} - 1.03 \ln \left(\frac{2}{V_1/V_2 + 1}\right).$$

Note that $\chi_{\text{QBCCA}}$ approaches to $\chi_{\text{BCCA}}$ in the BCCA limit ($V_1/V_2 \rightarrow 1$) as must be by the definition of BCCA. Equation (19) does not reproduce the void factor in the BPCA limit ($V_1/V_2 \rightarrow \infty$). To bridge the gap between the BCCA and BPCA limit, OTS09 considered a formula

$$\chi = \min(\chi_{\text{QBCCA}}(V_1/V_2), \chi_{\text{BPCA}}).$$

It is easy to check that Equation (20) approaches to $\chi_{\text{BCCA}}$ and $\chi_{\text{BPCA}}$ in the BCCA and BPCA limits, respectively. Equation (20) will be used in the numerical simulations presented in Section 4 to determine the porosity (volume) of aggregates after collisions.

#### 2.3.2. Projected Area

The projected area $A$ is another key property of porous aggregates. This does not affect only the charge state of the gas–dust mixture (Equation (4)) but also the drift velocity of individual aggregates (Equation (10)).

For BCCA clusters, the projected area averaged for fixed $N$ is well approximated by (Minato et al. 2006)

$$\bar{A}_{\text{BCCA}} = \pi a_0^2 \times \begin{cases} 12.5 N^{0.685} \exp(-2.53 N^{0.0920}), & N < 16, \\ 0.352 N + 0.566 N^{0.862}, & N \geq 16. \end{cases}$$

(21)

For BPCA clusters, the averaged projected area is simply related to the radius as $\bar{A}_{\text{BPCA}} \approx \pi a^2$. For more general porous aggregates, including QBCCA clusters, the averaged projected area is well approximated by (Equation (47) of OTS09)

$$\bar{A} = \left(\frac{1}{\bar{A}_{\text{BCCA}}(N)} + \frac{1}{\pi a^2} - \frac{1}{\pi a_{\text{BCCA}}(N)^2}\right)^{-1},$$

(22)

where $a$ and $N$ are the characteristic radius and monomer number of the aggregate considered, and $a_{\text{BCCA}}(N)$ and $\bar{A}_{\text{BCCA}}(N)$ are the characteristic radius and projected area of BCCA clusters with the same monomer number $N$ (i.e., Equations (18) and (21)), respectively. Note that the above formula reduces to
Equation (21) in the BCCA limit \((a \approx a_{\text{BCCA}})\) and to \(A \approx \pi a^2\) in the BPCA limit \((a \ll a_{\text{BCCA}}, \pi a^2 \ll A_{\text{BCCA}})\).

It should be noted that the above formulae can be only used for the average value of \(A\). This does not bother us when we compute the charge state of aggregates, since it only depends on the total projected area \(A_{\text{tot}}\). However, we cannot ignore the dispersion of \(A\) when we calculate the differential drift velocity between aggregates, especially between BCCA-like clusters. For example, let us consider two BCCA clusters with different masses \(N_1\) and \(N_2 (\neq N_1)\). As Equation (21) suggests, the mean mass-to-area ratio \(N/A_{\text{BCCA}}\) of BCCA clusters approaches to a constant value in the limit of large \(N\). Hence, if we ignore the area dispersion, we would have a differential drift velocity \(\Delta u_D \propto \Delta(N/A)\) vanishing for very large \(N_1\) and \(N_2\) even if \(N_1 \neq N_2\). Clearly, this would lead to underestimation of \(\Delta u_D\) and overestimation of the electrostatic repulsion.

To avoid this problem, we should replace \(|N_1/A_1 - N_2/A_2|^2\) in \(\mathcal{E}_D\) with \(|\overline{N}_1/A_1 - \overline{N}_2/A_2|^2\), not with \(|N_1/A_1 - N_2/A_2|^2\), where the overlines denote the statistical average. In particular, if the standard deviation of \(N/A\) scales linearly with its mean, we can write \([\Delta(N/A)]^2\) as (see the Appendix)

\[
[\Delta(N/A)]^2 = |\overline{N}_1/A_1 - \overline{N}_2/A_2|^2 + \varepsilon^2 \sum_{j=1,2} (N_j/A_j)^2, \tag{23}
\]

where \(\varepsilon\) is the ratio of the standard deviation to the mean of \(N/A\). In the Appendix, we evaluate \(\varepsilon\) from the numerical data on the projected area of sample BCCA clusters. We find that \(\varepsilon\) can be well approximated as \(\sim 0.1\) for \(N \lesssim 10^6\). In the following sections, we will assume \(\varepsilon = 0.1\) for all aggregates, since the area dispersion is only important for collision between BCCA-like clusters.

### 2.4. Nondimensionalization

As seen above, our dust model is characterized by a number of model parameters. To find a truly independent set of model parameters, we scale all the physical quantities involved into dimensionless ones.

We introduce the dimensionless radius and mean projected area,

\[
R \equiv \frac{a}{a_0}, \quad A \equiv \frac{A}{\pi a_0^2}. \tag{24}
\]

Also, we scale the mass \(M\) with the monomer number \(N = M/m_0\), where \(m_0\) is the mass of monomers. The normalized drift energy \(\mathcal{E}_D\) and electrostatic energy \(\mathcal{E}_E\) are already given by Equations (14) and (15), respectively. Using \((R, A, N)\) instead of \((a, A, M)\), we have

\[
\mathcal{E}_D = f_D \frac{N_1 N_2}{N_1 + N_2} \left[ \frac{N_1}{A_1} - \frac{N_2}{A_2} \right]^2 + \varepsilon^2 \sum_{j=1,2} \left( \frac{N_j}{A_j} \right)^2, \tag{26}
\]

\[
\mathcal{E}_E = f_E \left( \frac{\Psi}{\Psi_\infty} \right)^2 \frac{R_1 R_2}{R_1 + R_2}, \tag{27}
\]

where the dimensionless coefficients \(f_D\) and \(f_E\) are defined as

\[
f_D \equiv \frac{m_0}{2k_B T} \left( \frac{g \rho_0 a_0}{\rho_g \sqrt{8 k_B T}} \right)^2 = 1.7 \times 10^{-5} \left( \frac{\rho_0}{0.1 \mu m} \right) \left( \frac{1 \text{ g cm}^{-3}}{10^{-3} \text{ cm s}^{-2}} \right)^2 \times \left( \frac{\rho_g}{10^{-11} \text{ g cm}^{-3}} \right)^2 \left( \frac{T}{100 \text{ K}} \right)^{-2}, \tag{28}
\]

\[
f_E \equiv \frac{a_0 \Psi_\infty^3 k_B T}{e^2} = 0.60 \Psi_\infty^2 \left( \frac{\rho_0}{0.1 \mu m} \right) \left( \frac{T}{100 \text{ K}} \right), \tag{29}
\]

with the monomer material density \(\rho_0 = 3 m_0/4 \pi a_0^3\). We also introduce the normalized distribution function

\[
\mathcal{F}(N) = \frac{n(M) dM}{n_0}, \tag{30}
\]

where \(n_0\) is the number density of monomers in the initial state. Note that the mass conservation \(\int M n(M) dM = m_0 n_0\) can be written as \(\int \mathcal{F}(N) dN = 1\). Using \(\mathcal{F}\), we rewrite the ionization parameter \(\Theta\) as

\[
\Theta = \frac{h \Psi_\infty}{A_{\text{tot}} c_{\text{tot}}}, \tag{31}
\]

where \(A_{\text{tot}} \equiv \int A(N) \mathcal{F}(N) dN\) and \(c_{\text{tot}} \equiv \int (R(N)) \mathcal{F}(N) dN\) are the normalized total projected area and capacitance, and \(h\) is a dimensionless ionization rate defined by

\[
h \equiv \frac{\zeta \Psi_\infty^2}{\pi a_0^3 n_0^2 \Psi_\infty k_B T \sqrt{\pi m_0}} = 8.1 \times 10^{-3} \Psi_\infty \left( \frac{\rho_0}{0.1 \mu m} \right) \left( \frac{\rho_g}{10^{-11} \text{ g cm}^{-3}} \right)^{-1} \left( \frac{T}{100 \text{ K}} \right)^{-3/2} \left( \frac{\zeta}{10^{-17} \text{ s}^{-1}} \right). \tag{32}
\]

The surface potential \(\Psi\) is determined as a function of \(\Theta\) by Equation (3), or

\[
\frac{1}{1 + \Psi} - \exp (\Psi - \Psi_\infty) + \frac{A_{\text{tot}} c_{\text{tot}}}{h} \frac{\Psi}{\Psi_\infty} = 0, \tag{33}
\]

where we have eliminated \(s_i u_i/s_o u_o\) using Equation (6).

From the above scaling, we find that the collisional growth of charged dust aggregates can be characterized by five dimensionless parameters \((f_D, f_E, h, \varepsilon, \Psi_\infty)\).

### 3. MONODISPERSE GROWTH MODEL

Before proceeding to the full simulations, we consider simplified situations where dust grows into monodisperse aggregates, i.e., where all the aggregates have the same monomer number \(N\) at each moment. This greatly helps us to understand the results of the numerical simulations shown in the following section.

Within the framework of the hit-and-stick aggregation model, the monodisperse growth is equivalent to the BCCA growth. Thus, the assumption of the monodisperse growth is expressed by the following relations:

\[
a = a_0 \left( \frac{M}{m_0} \right)^{1/D} \iff R = N^{1/D}, \tag{34}
\]

\[
A = A_{\text{BCCA}}(N) \iff A = A(N) \equiv \frac{A_{\text{BCCA}}(N)}{\pi a_0^2}, \tag{35}
\]

\[
\mathcal{F}(N) = \frac{n(M) dM}{n_0}, \tag{30}
\]

where \(n_0\) is the number density of monomers in the initial state. Note that the mass conservation \(\int M n(M) dM = m_0 n_0\) can be written as \(\int \mathcal{F}(N) dN = 1\). Using \(\mathcal{F}\), we rewrite the ionization parameter \(\Theta\) as

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where \(A_{\text{tot}} \equiv \int A(N) \mathcal{F}(N) dN\) and \(c_{\text{tot}} \equiv \int (R(N)) \mathcal{F}(N) dN\) are the normalized total projected area and capacitance, and \(h\) is a dimensionless ionization rate defined by

\[
\frac{1}{1 + \Psi} - \exp (\Psi - \Psi_\infty) + \frac{A_{\text{tot}} c_{\text{tot}}}{h} \frac{\Psi}{\Psi_\infty} = 0, \tag{33}
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\]

\[
A = A_{\text{BCCA}}(N) \iff A = A(N) \equiv \frac{A_{\text{BCCA}}(N)}{\pi a_0^2}, \tag{35}
\]
Here, we give some examples to show how $\mathcal{E}_K$ and $\mathcal{E}_D$ depend on the parameters. Figure 4 shows $\mathcal{E}_K$ as a function of $N$ for $f_{D}\epsilon^2 = 10^{-7}$. As found from this figure, the kinetic energy is constant at $N \lesssim 10^5$ due to Brownian motion ($\mathcal{E}_K \approx 1$) and increases with mass at $N \gtrsim 10^6$ due to the differential drift ($\mathcal{E}_K \approx \mathcal{E}_D \propto N^3/A$). The qualitative behavior is the same for every $f_{D}\epsilon^2$. The value of $f_{D}\epsilon^2$ only determines the mass at which the differential drift starts to dominate over Brownian motion in the kinetic energy. In Figure 4, we also plot $\mathcal{E}_K$ for $f_{E} = 10$ with varying the value of $h(= 10^{-4.5}, 10^{-6}, 10^{-7.5})$. For all the cases, $\mathcal{E}_K$ quickly increases with $N$ and finally becomes proportional to $R = N^{1/2}$. This reflects the transition of the plasma state from the IDP ($\Psi \approx \Theta \propto N^{3/2}/A$) to the IEP ($\Psi \approx \Psi_\infty$). In the IEP limit, $\mathcal{E}_E$ depends on $f_{D}$ but is independent of $h$. An important difference among the three examples is the timing of the plasma transition: for smaller $h$, $\mathcal{E}_E$ approaches the IEP limit at larger $N$. This difference makes the ratio between $\mathcal{E}_E$ and $\mathcal{E}_K$ quantitatively different among the three cases. For $h = 10^{-4.5}$, $\mathcal{E}_E$ exceeds $\mathcal{E}_K$ when the relative motion is dominated by Brownian motion. For $h = 10^{-6}$, by contrast, $\mathcal{E}_E$ exceeds $\mathcal{E}_K$ when the relative motion is dominated by the differential drift. For $h = 10^{-7.5}$, $\mathcal{E}_E$ does not exceed $\mathcal{E}_K$ for arbitrary $N$. As we see in Section 4, this difference is a key to the understanding of the collisional growth of dust aggregates with size distribution.

To quantify these differences for general cases, we introduce the following quantities.

1. The drift mass $N_D$. This is defined as the mass at which the relative motion starts to be dominated by the differential drift.

2. The plasma transition mass $N_F$. This is defined as the mass at which the plasma state shifts from the IDP to the IEP.

3. The maximum energy ratio $(\mathcal{E}_E/\mathcal{E}_K)_{\text{max}}$. This is the maximum value of the ratio $\mathcal{E}_E/\mathcal{E}_K$ in the monodisperse growth. If $(\mathcal{E}_E/\mathcal{E}_K)_{\text{max}} > 1$, the electrostatic energy $\mathcal{E}_E$ exceeds the kinetic energy $\mathcal{E}_K$ at a certain mass.

4. The freezeout mass $N_F$. This is the mass at which $\mathcal{E}_E$ starts to exceed $\mathcal{E}_K$. Note that the freezeout mass is only defined when $(\mathcal{E}_E/\mathcal{E}_K)_{\text{max}} > 1$.

In the following subsection, we describe how these quantities are related to the parameters ($f_{D}\epsilon^2, f_{E}, h$).

### 3.1. $N_D$: the Drift Mass

The first and second terms on the right-hand side of Equation (39) represent Brownian motion and the differential drift. Since the second term monotonically increases with $N$, there exists a critical mass at which the dominant relative motion changes from the Brownian motion to the differential drift. We define $N_D$ as the critical mass satisfying $\mathcal{E}_D(N_D) = 1$. Using Equation (37), the equation for $N_D$ is written as

$$\frac{A(N_D)^2}{N_D^3} = f_{D}\epsilon^2. \tag{40}$$

This equation implicitly determines $N_D$ as a function of $f_{D}\epsilon^2$. For example, $N_D \approx 3 \times 10^4$ when $f_{D}\epsilon^2 = 10^{-7}$ (see Figure 4).

Figure 5 shows the solution to Equation (40). When $f_{D}\epsilon^2 \ll 1$, $N_D$ is well approximated as

$$N_D \approx \frac{1}{b^2 f_{D}\epsilon^2}, \tag{41}$$

where $b$ is determined from Equations (37) and (39).
where \( b = 1/0.352 = 2.84 \) is the mass-to-area ratio \( N/A(N) \) in the limit of \( N \to \infty \). Using Equation (41), \( \xi_K \) is simply rewritten as

\[
\xi_K \approx 1 + \frac{N}{N_D},
\]

which asymptotically behaves as \( \xi_K \approx 1 \) for \( N \ll N_D \) and \( \xi_K \approx N/N_D \) for \( N \gg N_D \). The asymptotic form of \( \xi_K \) is schematically illustrated in Figure 6(a).

### 3.2. \( N_P \): the Plasma Transition Mass

Another important quantity is the critical mass at which the plasma state changes from IDP to IEP. We define the critical mass \( N_P \) such that \( \Theta(N_P) = \Psi_{\infty} \) (see Equation (5)). Using Equation (31), this condition can be written as

\[
\frac{A(N_P)}{N_P^{3/2}} = h.
\]

Note that \( N_P \) depends on \( h \) only.

Figure 5 shows the solution to Equation (43) as a function of \( h \). If \( h \ll 1 \), \( N_P \) is well approximated as

\[
N_P \approx \frac{1}{b^2 h^2}.
\]

In this case, \( \xi_E \) can be approximately written as

\[
\xi_E \approx \frac{f_E}{2} \left[ 1 + \left( \frac{N}{N_P} \right)^{-0.4} \right]^{-2.5} N^{1/2},
\]

which asymptotically behaves as \( \xi_E \approx (f_E/2)N^{3/2}/N_P \) for \( N \ll N_P \) and as \( \xi_E \approx (f_E/2)N^{1/2} \) for \( N \gg N_P \). The asymptotic form of \( \xi_E \) is illustrated in Figure 6(b).

### 3.3. \( \xi_E/\xi_K \) max: the Maximum Energy Ratio

The maximum energy ratio \( \xi_E/\xi_K \) max determines whether the electrostatic energy exceeds the kinetic energy during the monodisperse growth. Since \( \xi_E \) scales linearly with \( f_E \), the quantity \( f_E^{-1}(\xi_E/\xi_K)_{\text{max}} \) depends only on \( f_D \epsilon^2 \) and \( h \).

Figure 7 plots \( f_E^{-1}(\xi_E/\xi_K)_{\text{max}} \) as a function of \( f_D \epsilon^2 \) and \( h \). It is seen that the maximum energy ratio behaves differently across the line \( N_D = N_P \). This can be easily understood from Figure 8, which schematically illustrates the mass dependence of \( \xi_K \) and \( \xi_E \) (Equations (42) and (45)). If \( N_D \gg N_P \) \( (f_D \epsilon^2 \ll h^2) \), the energy ratio \( \xi_E/\xi_K \) reaches the maximum at \( N \approx N_D \). Since \( \xi_K(N_P) = 2 \) and \( \xi_E(N_P) \approx f_E N_P^{1/2} / 2 \), we obtain \( (\xi_E/\xi_K)_{\text{max}} \approx f_E N_P^{1/2} / 4 \approx f_E / 4 b f_D \epsilon \) independently of \( h \). If \( N_D \ll N_P \) \( (f_D \epsilon^2 \gg h^2) \), by contrast,
\[ \frac{E_{E}}{E_{K}} \text{ reaches the maximum at } N \approx N_{P}. \] Using \( E_{K}(N_{P}) \approx N_{P}/N_{D} \) and \( E_{E}(N_{P}) \approx f_{E}N_{P}^{1/2}/2^{1.5} \), we have \( \frac{E_{E}/E_{K}}{\text{max}} \approx f_{E}N_{P}^{1/2}/2^{1.5}N_{P} \approx f_{E}h/2^{1.5}b_{D}e^{2} \), which depends on both \( b_{D}e^{2} \) and \( h \).

### 3.4. NF: the Freezeout Mass

When \( \left( \frac{E_{E}/E_{K}}{\text{max}} \right) > 1 \), there exists a critical mass \( N_{F} \) at which the electrostatic energy \( E_{E} \) takes over the kinetic energy \( E_{K} \). As we will see in Section 3.5, the monodisperse growth is strongly suppressed at \( N \gtrsim N_{F} \). For this reason, we refer to \( N_{F} \) as the “freezeout mass.” The freezeout mass can be calculated from the condition \( E_{E}(N_{F}) = E_{E}(N_{P}) \) once the three parameters \( f_{D}e^{2}, f_{E}, \) and \( h \) are specified.

In Figure 9, we plot \( N_{F} \) as a function of \( f_{D}e^{2} \) and \( h \) for \( f_{E} = 10 \). We see that \( N_{F} \) depends on these parameters differently depending on the values of \( E_{E}(N_{P}) \) and \( E_{E}(N_{D}) \). To understand this, in Figure 10, we schematically show \( E_{K} \) and \( E_{E} \) as a function of \( N \) for the three cases. If \( E_{E}(N_{D}) \gtrsim 1, E_{E} \) starts to exceed \( E_{K} \) when the relative velocity is dominated by Brownian motion (i.e., \( N_{F} \ll N_{D} \)). In this case, the condition determining \( N_{F} \) is given by \( E_{E}(N_{F}) \approx 1 \), which implies \( N_{F} \approx (2/f_{E})^{2} \) for \( E(N_{P}) \ll 1 \) and \( N_{F} \approx (2N_{P}/f_{E})^{2/3} \approx (2h^{2}f_{D}e^{2}N_{P})^{2/3} \) for \( E(N_{P}) \gtrsim 1 \). If \( E_{E}(N_{D}) \ll 1 \) but still \( \left( \frac{E_{E}/E_{K}}{\text{max}} \right) > 1 \), \( E_{E} \) exceeds \( E_{K} \) after the relative velocity is dominated by the differential drift (i.e., \( N_{F} \gg N_{D} \)). In this case, the condition for \( N_{F} \) is given by \( (f_{E}/2)N_{P}^{1/2}/N_{P} \approx N_{F}/N_{D} \), hence \( N_{F} \) is given by \( N_{F} \approx (2N_{P}/f_{E}N_{D})^{2} \approx (2f_{D}e^{2}/f_{E}h^{2})^{2} \).

### 3.5. The Outcomes of Monodisperse Growth

As mentioned above, the monodisperse growth is expected to slow down at the freezeout mass \( N \approx N_{F} \) when \( \left( \frac{E_{E}/E_{K}}{\text{max}} \right) > 1 \). Here, we demonstrate this by numerically calculating the mass evolution.
Under the monodisperse approximation, the evolution of aggregate mass $N$ is given by

$$\frac{dM}{dt} = \rho_d K \Leftrightarrow \frac{dN}{dT} = \mathcal{K},$$

where $T = n_0 \pi a_0^3 \sqrt{8k_B T / \pi m_0}$ and $\mathcal{K} = K / (\pi a_0^3 \sqrt{8k_B T / \pi m_0})$ are the dimensionless time and collisional rate coefficient. We numerically solve Equation (46) with initial condition $N(T = 0) = 1$.

As in the beginning of this section, we consider three cases of $h = 10^{-4.5}$, $10^{-6}$, and $10^{-7.5}$ with fixed $f_D e^2 = 10^{-2}$ and $f_E = 10$. Listed in Table 1 are the critical masses $(N_D, N_P, N_F)$ and the maximum energy ratio $(\mathcal{E}_E / \mathcal{E}_K)_{\text{max}}$ for these cases. We also consider the uncharged case with the same value of $f_D e^2$.

### 3.5.1. Without Charging

In Figure 11, the mass evolution for the uncharged case is shown by the dashed curve. The black arrow in the figure indicates the critical drift mass $N_D = 10^{9.3}$. We find that the mass grows as $T^2$ until reaching $N_D$, and then grows exponentially with $T$. This evolutionary trend can be directly proven from Equation (46). Without charging, the collision kernel $\mathcal{K}$ is just the product of the geometrical cross section $\propto R^2 = N$ and the relative velocity $\Delta u$. When $N \ll N_D$, the relative velocity is dominated by Brownian motion (i.e., $\Delta u \propto N^{-1/2}$), and we have $\mathcal{K} \propto R^2 N^{-1/2} \propto N^{1/2}$. Inserting this into Equation (46), we have $N \propto T^2$. When $N \gg N_D$, by contrast, the relative velocity is dominated by the differential drift ($\Delta u \propto N^{-1/3}$), and hence $\mathcal{K} \propto N^{2/3} / A$. Since the projected area $A$ roughly scales with $R^2$, we have $\mathcal{K} \propto N$. Hence, from Equation (46), we find $N \propto \exp(\Omega T)$, where $\Omega$ is a constant growth rate.

### 3.5.2. With Charging

The mass evolution for the charged cases is plotted in Figure 11 by gray curves. The gray arrows in the figure indicate the freezeout mass $N_F$ for $h = 10^{-4.5}$ and $10^{-6}$. As expected, we observe significant slowdown in the growth at $N \approx N_F$ for the two cases. At $T = 10^4$, the aggregate mass is $N \approx 10^{8.7}$ for $h = 10^{-4.5}$ and $N \approx 10^{8.9}$ for $h = 10^{-6}$, which is consistent with the predicted freezeout mass (see Table 1). We have computed the mass evolution for the two cases until $T = 10^6$, but the final masses $10^{8.9}$ and $10^{9.0}$ are not very different from the values at $T = 10^4$.

For $h = 10^{-7.5}$, by contrast, the evolution curve of $N$ is indistinguishable from that for the uncharged case, meaning that the electrostatic repulsion hardly affects the aggregate growth. To summarize, we have confirmed that dust can continue the monodisperse growth only if

$$\left(\frac{\mathcal{E}_E}{\mathcal{E}_K}\right)_{\text{max}} \lesssim 1.$$

### 4. NUMERICAL SIMULATIONS INCLUDING SIZE DISTRIBUTION

As shown in the previous section, dust aggregates could not grow beyond the freezeout mass $N_F$ if condition (47) is not satisfied and if the size distribution were limited to monodisperse ones. In this section, we study how the outcome of dust growth changes when we allow the size distribution to freely evolve.

To compute the evolution of the size distribution, we employ the “extended” Smoluchowski method developed in OTS09. This method treats the number density $n(M)$ and the mean volume $\overline{V}(M)$ of aggregates with mass $M$ as time-dependent quantities, and calculates their temporal evolution simultaneously. This method allows us to follow the porosity evolution consistently with collisional growth, which cannot be done with the conventional Smoluchowski method (e.g., Nakagawa et al. 1981; Tanaka et al. 2005; Dullemond & Dominik 2005).

In the extended Smoluchowski method, the temporal evolution of $n(M)$ and $\overline{V}(M)$ is given by two equations

$$\frac{\partial n(M)}{\partial t} = \frac{1}{2} \int_0^M dM' \left\{ \overline{K}(M'; M - M') n(M') n(M - M') - n(M) \int_0^{\infty} dM'' \overline{K}(M'; M - M') n(M'), \right\},$$

$$\frac{\partial [\overline{V}(M) n(M) ]}{\partial t} = \frac{1}{2} \int_0^M dM' \left\{ \overline{V}_{1+2}(M'; M - M') \times \overline{K}(M'; M - M') n(M') n(M - M') - \overline{V}(M) n(M) \int_0^{\infty} dM'' \overline{K}(M'; M - M') n(M'), \right\},$$

where $\overline{K}(M_1; M_2)$ and $\overline{V}_{1+2}(M_1; M_2)$ are the collisional rate coefficient $K$ (Equation (12)) and the aggregate volume $V_{1+2}$ after a collision (Equation (17)) evaluated for $V_1 = \overline{V}(M_1)$ and $V_2 = \overline{V}(M_2)$. In this study, we determine $V_{1+2}$ using the formula for hit-and-stick collisions (Equation (20)).

| $h$    | $N_D$  | $N_P$  | $(\mathcal{E}_E / \mathcal{E}_K)_{\text{max}}$ | $N_F$  |
|--------|--------|--------|---------------------------------|--------|
| $10^{-4.5}$ | $10^6$  | $10^{9.3}$ | $10^{10.3}$ | $10^{7.5}$  |
| $10^{-6}$  | $10^6$  | $10^{9.1}$ | $10^{9.5}$  | $10^{8.8}$  |
| $10^{-7.5}$ | $10^6$  | $10^{9.1}$ | $10^{1-10}$ | $\ldots$   |

Figure 11. Mass evolution in the monodisperse model calculated from Equation (46) for $f_D e^2 = 10^{-7}$ and $f_E = 10$ with various values of $h$. The black arrow indicates the drift mass $N_D$, while the lower and upper arrows show the freezeout mass $N_F$ for $h = 10^{-4.5}$ and $10^{-6}$, respectively. The evolution for the uncharged case (i.e., $h = 0$) is shown by the dashed curve.
We numerically solve Equations (48) and (49) using the fixed bin scheme described in OTS09. This scheme divides the low-mass region $m_0 \leq M \leq N_{bd} m_0$ into linearly spaced bins with representative masses $M_k = k m_0 (k = 1, 2, \ldots, N_{bd})$ and the high-mass region $M > N_{bd} m_0$ into logarithmically spaced bins with $M_k = 10^{1/2} N_{bd} M_{k-1} (k = N_{bd} + 1, \ldots)$. The number $N_{bd}$ controls the resolution in the mass coordinate. In this study, we set $N_{bd} = 80$ (meaning $M_{k+1}/M_k = 1.03$ for the high-mass range). The temporal evolution is computed using the explicit, fourth-order Runge–Kutta method. The time increment $\Delta t$ for each time step is continuously adjusted so that the fractional decrease in the number density during $\Delta t$ does not exceed $\delta t$ for all bins, where $\delta t$ is a constant parameter. We take $\delta t = 0.02$ in the following calculations.

4.1. Without Charging

Figure 12 shows the solution to Equations (48) and (49) for the uncharged case of $(f_{pe}^2, \epsilon) = (10^{-7}, 10^{-1})$. The upper panel displays the mass distribution function $F(N)$ at various times $T$. Note that the vertical axis of this panel is chosen to be $N^2 F(N)$, which is proportional to the mass density of aggregates belonging to each logarithmic mass bin.

To characterize the evolution of the mass distribution, we introduce the average mass $\langle N \rangle$ and the mass-weighted average mass $\langle N \rangle_m$ defined by

$$
\langle N \rangle \equiv \int_0^\infty N F(N) dN = \frac{1}{\int_0^\infty F(N) dN},
$$

$$
\langle N \rangle_m \equiv \int_0^\infty N^2 F(N) dN = \int_0^\infty N^2 F(N) dN,
$$

where we have used the mass conservation $\int_0^\infty N F(N) dN = 1$.

As pointed out by the referee, this is a general consequence of the kernel $K$ scaling linearly with the masses of colliding aggregates (this is the case for our kernel at $N > N_D$, see Section 3.5.1). In fact, the growth rate of $\langle N \rangle_m$ is known to be exactly twice as high as that of $\langle N \rangle$ when the kernel is of the form $K(N_1; N_2) \propto N_1 + N_2$ (see, e.g., Figure 1 of Ormel & Spaans 2008).

Figure 12. Evolution of the mass distribution function $F(N)$ (upper panel) and the mass–radius relation $R(N)$ (lower panel) for the uncharged case of $(f_{pe}^2, \epsilon) = (10^{-7}, 10^{-1})$. The gray curves show the snapshots of $N^2 F(N)$ and $R(N)$ at various times, $T = 10^4, 10^5, 10^6, \ldots, 10^8$ (from left to right). Note that the curves for $R(N)$ overlap each other. The arrows indicate the critical mass $N_0$ calculated from the monodisperse theory (Equation (40)). The crosses and open circles in the upper panel indicate the averaged mass $\langle N \rangle$ (Equation (50)) and the weighted averaged mass $\langle N \rangle_m$ (Equation (51)), respectively. In the lower panel, the mass–radius relations for the fractal dimensions of $D = 2$ and 3 are shown by the dashed and dotted curves, respectively.

4.2. With Charging

Now we show how the charging alters the evolution of the size distribution. As in Section 3, we consider three cases of
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Figure 13. Same as the upper panel of Figure 12, but for three charged cases, \( h = 10^{-4.5}, 10^{-6}, \) and \( 10^{-7.5} \) (from top to bottom). The other parameters are set to \( (f_D \epsilon^2, f_E, \epsilon, \Psi) = (10^{-7}, 10, 10^{-1}, 10^6) \). The gray arrows indicate the freezeout mass \( N_F \) predicted from the monodisperse theory. The dotted curves in the middle and bottom panels show the mass distribution when the surface potential \( \Psi \) exceeds the critical value \( \Psi^\star \) (Equation (53)).

\[ h = 10^{-4.5}, 10^{-6}, \text{and } 10^{-7.5} \text{ with } (f_D \epsilon^2, f_E, \epsilon) = (10^{-7}, 10, 10^{-1})\).

In Figure 13, we show the temporal evolution of the mass distribution \( J(N) \) for the three cases. The mass–radius relation \( R(N) \) is not shown here because it is very similar to that for the uncharged case. For \( h = 10^{-4.5} \), the monodisperse theory gives \( (E_k/E_k)_{\text{max}} > 1 \), predicting the freezeout of the growth at \( N \approx N_F \approx 10^5 \) (see Table 1). As expected, the evolution of the mass distribution starts to slow down at \( N \approx N_F \), ending up with nearly monodisperse distribution peaked at \( N \approx 10^6 \). In the simulation, we have followed the evolution at \( T = 10^6 \), but observed no significant growth after \( T > 10^4 \).

For \( h = 10^{-6} \) and \( 10^{-7.5} \), by contrast, the outcome is qualitatively different from the prediction by the monodisperse theory, as is shown in the middle and bottom panels of Figure 13, respectively. For the case of \( h = 10^{-6} \), the prediction was that the freezeout occurs at \( N \approx N_F \approx 10^5 \). However, the simulation shows the size distribution evolving into a bimodal distribution, in which one peak stays at \( N \approx N_D \) and the other continues growing toward larger \( N \). Interestingly, similar behavior is seen in the case of \( h = 10^{-7.5} \) despite the fact that the charging did not affect dust growth for this case within the monodisperse theory.

The evolution of the size dispersion can be better understood if we look at the evolution of \( \langle N \rangle \) and \( \langle N \rangle_m \). Figure 14 compares them among the three charged cases together with the uncharged case. See also Figure 11 in which the prediction from the monodisperse theory is shown. For \( h = 10^{-4.5} \), both \( \langle N \rangle \) and \( \langle N \rangle_m \) evolves as the monodisperse theory predicts. However, for \( h = 10^{-6} \) and \( 10^{-7.5} \), \( \langle N \rangle \) stops growing at certain values, while \( \langle N \rangle_m \) continues growing as for the uncharged case. This means that, in the latter cases, only a small number of aggregates continue growing but nevertheless carry the greater part of dust mass in the system.

As we explain below, the transition to the bimodal distribution can be characterized by three steps.

1. At \( \langle N \rangle_m > N_D \), a long tail is formed at the low-mass end of the size distribution.
2. Since aggregates belonging to the low-mass tail have a relatively small kinetic energy, they stop growing as the surface potential \( \Psi \) reaches a certain value \( \Psi^\star \) (see Equation (53) below). These “frozen” aggregates provide the total capacitance \( C_{\text{tot}} \), which no longer decreases with time. This leads to the surface potential \( \Psi \) of all aggregates no longer increasing with time.
3. Consequently, aggregates of higher mass are less charged than in the case of the monodisperse growth. The growth of the high-mass aggregates is no longer inhibited by the charge barrier.

Figure 14. Evolution of the average mass \( \langle N \rangle \) (upper panel) and the weighted average mass \( \langle N \rangle_m \) (lower panel) as a function of time \( T \). The gray curves indicate the results for three charged cases of \( h = 10^{-4.5}, 10^{-6}, 10^{-7.5} \), while the black dashed curves are for the uncharged case \( (h = 0) \). The other parameters are set to \( (f_D, f_E, \epsilon, \Psi^\star) = (10^{-5}, 10, 10^{-1}, 10^6) \). The gray and black arrows indicate the critical drift mass \( N_D \) and the freezeout mass \( N_F \) predicted by the monodisperse theory, respectively.
The first step was already discussed in the previous subsection. Here, we explain how the second step follows after the development of the low-mass tail. Let us approximate the mass distribution at the end of the first stage into two subgroups, one representing the high-mass side and the other representing the low-mass tail. We characterize them with masses $N_1 \gg N_D$ and $N_2 \approx N_D$. The number of the low-mass aggregates decreases through their mutual collisions ("2–2 collision") and through sweep-up by the high-mass aggregates ("1–2 collision"). This leads to the decrease in the total capacitance $C_{\text{tot}}$ and, in turn, the increase in the surface potential $\Psi$. We now write the relative kinetic energies for 1–2 and 2–2 collisions as $\varepsilon_{K,12}$ and $\varepsilon_{K,22}$. Using Equations (26), (39), and (40) together with $N/A \approx b$ and $N_1 \gg N_2 \approx N_D$, these energies are approximately evaluated as $\varepsilon_{K,12} \approx 1 + 2N_2/N_D \approx 3$ and $\varepsilon_{K,22} \approx 1 + N_2/N_D \approx 2$, respectively. Note that $\varepsilon_{K,12}$ is nearly independent of $N_1$ because the reduced mass is determined by smaller aggregates and because the drift velocity $\propto N_1/A_1$ is nearly constant at large $N_1$. Meanwhile, the electrostatic energies (Equation (27)) for 1–2 and 2–2 collisions are written as $\varepsilon_{E,12} \approx f_{\text{E}}(\Psi/\Psi_\infty)^2 R_2 \approx f_{\text{E}}(\Psi/\Psi_\infty)^2 N_D / 2$ and $\varepsilon_{E,22} \approx f_{\text{E}}(\Psi/\Psi_\infty)^2 R_2 / 2 \approx f_{\text{E}}(\Psi/\Psi_\infty)^2 N_{D/2}^2 / 2$, respectively. Again, $\varepsilon_{E,12}$ is independent of $N_1$, because the reduced radius is determined by smaller aggregates. Thus, the energy ratios for 1–2 and 2–2 collisions are obtained as

$$\frac{\varepsilon_{E,12}}{\varepsilon_{K,12}} \approx \frac{f_{\text{E}} \Psi^2 N_D^{1/2}}{3 \Psi_\infty^{1/2}}, \quad \frac{\varepsilon_{E,22}}{\varepsilon_{K,22}} \approx \frac{f_{\text{E}} \Psi^2 N_{D/2}^{1/2}}{4 \Psi_\infty^{1/2}},$$

independently of $N_1$. Both the energy ratios exceed unity when $\Psi \gtrsim \Psi_\infty^*$, where

$$\Psi_\infty^* \equiv \left( \frac{4}{f_{\text{E}} N_D^{1/2}} \right)^{1/2} \Psi_\infty \approx 2 \left( \frac{b f_{\text{E}}^{1/2}}{f_{\text{E}}} \right)^{1/2} \Psi_\infty^*.$$  \hspace{1cm} (52)

Note that $\Psi_\infty^*$ is independent of $h$. For $f_{\text{D}} e^2 = 10^{-7}$ and $f_{\text{E}} = 10$, we obtain $\Psi_\infty^* \approx 0.02 \Psi_\infty^\infty$. The above consideration suggests that the freezeout of the low-mass aggregates occurs when $\Psi$ exceeds the critical value $\Psi_\infty^*$. To confirm this, in the upper panel of Figure 15, we plot $\Psi$ versus the average mass $(N)$ for $h = 10^{-6}$ and $10^{-7.5}$. We see that the increase in $(N)$ stops when $\Psi$ exceeds $\Psi_\infty^*$. It should be noted that the evolution of $\Psi$ is also slowed down for $\Psi \gtrsim \Psi_\infty^*$. This is because the "frozen" small aggregates govern the total electric capacitance $C_{\text{tot}}$ of the system. Using $\Psi \approx \Theta \approx b h \Psi_\infty^\infty / C_{\text{tot}}$ (as is for the IDP limit), the total capacitance when $\Psi \approx \Psi_\infty^*$ can be evaluated as

$$C_{\text{tot}} \approx C_{\text{tot}, \infty} \equiv \frac{b h \Psi_\infty^\infty}{\Psi_\infty^*} \approx \frac{(b f_{\text{E}})^{1/2} h}{2 (f_{\text{D}} e^2)^{1/4}}.$$ \hspace{1cm} (54)

The values of $C_{\text{tot}, \infty}$ for the two cases are indicated in the lower right panel of Figure 15.

We are now able to explain why the high-mass aggregates can grow beyond $N \approx N_F$ in the case of $h = 10^{-6}$. First, note that they can grow only through their mutual collisions ("1–1 collision") because 1–2 collisions have already been inhibited. The relative kinetic energy and electrostatic energy for 1–1 collisions are given by $\varepsilon_{K,11} \approx 1 + N_1/N_D$ and $\varepsilon_{E,11} \approx (f_{\text{E}} / 2) (\Psi_*/\Psi_\infty^\infty)^2 N_1^{1/2}$. Using $N_1 \gg N_D$ and Equation (53), we obtain

$$\frac{\varepsilon_{E,11}}{\varepsilon_{K,11}} \approx \frac{f_{\text{E}} \Psi_*/\Psi_\infty^\infty N_D}{2 \Psi_\infty^\infty N_1^{1/2}} \approx 2 \left( \frac{N_D}{N_1} \right)^{1/2} \ll 1.$$ \hspace{1cm} (55)

Thus, we find that the energy ratio decreases with mass $N_1$, and therefore the growth of the high-mass aggregates is no longer inhibited by the charge barrier. This is essentially due to the frozen aggregates keeping the surface potential $\Psi$ nearly constant. Without the frozen aggregates, $\Psi$ would increase as $N_1^{1/2}$, and the electrostatic energy $\varepsilon_{E,11} \propto N_1^{1/2}$ would take over $\varepsilon_{K,11} \propto N_1$ at a certain mass as in the monodisperse case. With the frozen aggregates, by contrast, $\varepsilon_{E,11}$ increases only as $N_1^{1/2}$, so cannot exceed $\varepsilon_{K,11}$. It should be noted that the increasing kinetic energy will in reality cause collisional compaction at some stage, but this effect is neglected in our calculation.

One might wonder why the freezeout of the entire mass distribution occurs for $h = 10^{-4.5}$. The key difference between the two cases $h = 10^{-4.5}$ and $h = 10^{-6}$ is the timing at which the electrostatic barrier becomes effective. In the former case, the charge barrier becomes effective when the relative motion between aggregates is dominated by Brownian motion (i.e., $N_F < N_D$). In this case, the aggregates cannot overcome the barrier even if $\Psi$ is kept constant, since the electrostatic energy $\varepsilon_{E} \propto \Psi^2 N^{1/2}$ grows with mass while the kinetic energy $\varepsilon_{K} \approx 1$ does not. In the latter case, by contrast, the charge barrier becomes effective after the relative motion has been already dominated by the differential drift (i.e., $N_D < N_F$). In this case, the kinetic energy $\varepsilon_{K} \propto N$ can surpass the electrostatic energy if $\Psi$ is kept constant.

Finally, we remark that $\Psi_\infty^*$ can exceed $\Psi_\infty^\infty$ when $f_{\text{D}} e^2 / f_{\text{E}}^2$ is sufficiently large (see Equation (53)). In reality, however, the surface potential does not grow larger than $\Psi_\infty^\infty$. For such cases, the energy ratios in Equation (52) never exceed unity, so we expect that low-mass aggregates do not stop growing. We will confirm this expectation in the following subsection.
observed the total freezeout, bimodal growth, and unimodal growth, respectively. It is seen that the total freezeout occurs for small \( f_D \epsilon^2 \) and large \( h \), while the unimodal growth occurs when \( f_D \epsilon^2 \) is small.

First, we examine whether the total freezeout regime can be well represented by a criterion of the form \( \langle E_E/E_K \rangle_{\text{max}} > \text{constant} \) as suggested by the monodisperse theory (see Equation (47)). In Figure 16, we show a criterion \( \langle E_E/E_K \rangle_{\text{max}} > 3 \) with the solid curve. It is seen that this criterion applies well at large \( f_D \epsilon^2 \) while it overestimates the size of the freezeout region at smaller \( f_D \epsilon^2 \). It is clear that such a type of criteria do not explain the condition for the total freezeout to occur.

However, a criterion applicable for all parameter ranges can be obtained if we slightly modify Equation (47). The point is that the total freezeout is observed only in the Brownian motion regime, i.e., only when the freezeout mass \( N_F \) is smaller than the drift energy \( N_D \). This fact suggests that the total freezeout does not occur if \( \langle E_E/E_K \rangle_{\text{max}} > 1 \) but \( \langle E_E/N_D \rangle \ll 1 \) (this is the case for the parameter region (iii) in Figures 9 and 10). This expectation motivates us to introduce another energy ratio,

\[
\frac{\langle E_E/N_D \rangle}{\langle E_E/N_F \rangle} = 2,
\]

where we have used the definition of \( N_D \), i.e., \( E_K/N_D = 2 \).

Note that \( \langle E_E/N_D \rangle/2 \) is the maximum value of \( \langle E_E/E_K \rangle \) in the Brownian motion regime because \( E_E \) monotonically increases with \( N \) and \( E_K \leq 2 \) at \( N \leq N_D \). In Figure 16, we show the line \( \langle E_E/N_D \rangle = 6 \) with the dashed curve. We see that the line represents the boundary of the total freezeout regime very well. Thus, we conclude that the criterion for the total freezeout to occur is given by

\[
\langle E_E/N_D \rangle \gtrsim 6.
\]

A simple criterion is also obtained for the boundary between the bimodal and unimodal growth regimes. As mentioned in Section 4.2, the bimodal growth occurs only if the critical surface potential \( \Psi_c \) (Equation (53)) is lower than \( \Psi_\infty \). In Figure 16, we show the line \( \Psi_c = \Psi_\infty/4 \) with the dotted curve. We find that the condition for the bimodal growth to occur instead of the unimodal growth is given by

\[
\Psi_c \lesssim \Psi_\infty/4.
\]
To summarize, the outcome of charged dust growth can be classified into three cases (Table 2). If $\mathcal{E}_E(N_D) \gtrsim 6$, all aggregates stop growing before the systematic drift dominates their relative velocities. The outcome is a nearly monodisperse distribution of frozen aggregates with typical mass $\sim N_F$. If $\mathcal{E}_E(N_D) \lesssim 6$ and $\Psi_* \gtrsim \Psi_\infty/4$, a large number of aggregates stop growing, but a major part of mass within the system is carried by a small number of ever-growing aggregates. If $\mathcal{E}_E(N_D) \lesssim 6$ and $\Psi_* \gtrsim \Psi_\infty/4$, all aggregates continue growing with a single-peaked size distribution. The second case includes situations where no aggregates could continue growing if the size distribution were limited to a monodisperse one. This means that size distribution must be taken into account when we discuss how the charging of aggregates affects their collisional growth.

5. DISCUSSION

5.1. An Application to a Protoplanetary Disk Model

The growth criteria derived in Section 4 are general in a sense that no protoplanetary disk model is specified. Although application to particular disk models is the subject of Paper II, we will show here one example of how to use the criteria.

Here, we adopt the minimum-mass solar nebular (MMSN) model of Hayashi (1981). In this model, the gas temperature $T$ and the Kepler rotational frequency $\Omega_K$ are given by $T = 280(r/1 \text{ AU})^{-1/2} \text{ K}$ and $\Omega_K = (2\pi/1 \text{ yr})(r/1 \text{ AU})^{-3/2}$, where $r$ is the distance from the Sun. The gas density $\rho_g$ and the vertical component of the stellar gravity $g$ are given by $\rho_g = 1.4 \times 10^{-3}(r/1 \text{ AU})^{-11/4}\exp(-z^2/2H^2) \text{ g cm}^{-3}$ and $g = \Omega_K^2z = 0.020(r/1 \text{ AU})^{-1/2}(z/H)\text{ cm s}^{-2}$, where $z$ is the distance from the midplane of the disk. $H = c_s/\Omega_K = 5.0 \times 10^5(r/1 \text{ AU})^{1/4}$ is the gas scale height. In this subsection, we neglect the effect of disk turbulence to dust collision and assume the stellar gravity as the only source of dust differential drift. For the material density of monomers and the dust-to-gas mass ratio, we ignore the sublimation of ice for simplicity and set $\rho_i = 1.4 \text{ g cm}^{-3}$ and $\rho_i/\rho_g = 0.014$ (Tanaka et al. 2005). The maximum surface potential $\Psi_\infty$ is taken to be 2.81 as is for $m_i = 24m_H$ and $s_i = 0.3$. Substituting these relations into Equations (28), (29), and (32) and setting $z = H$, we obtain

$$f_D = 4.1 \times 10^{-5} \left( \frac{a_0}{0.1 \mu\text{m}} \right)^{5} \left( \frac{r}{5 \text{ AU}} \right)^{3},$$

$$f_E = 5.9 \left( \frac{a_0}{0.1 \mu\text{m}} \right) \left( \frac{r}{5 \text{ AU}} \right)^{-1/2},$$

$$h = 2.0 \times 10^{-3} \left( \frac{a_0}{0.1 \mu\text{m}} \right)^{3} \left( \frac{\zeta}{10^{-17} \text{ s}^{-1}} \right) \left( \frac{r}{5 \text{ AU}} \right)^{7/2}.$$ 

There equations give the radial profiles of $(f_D, f_E, h)$ for the MMSN model at one scale height above the midplane. In addition, we need to give the ionization rate $\zeta$ as a function of $r$. Here, we simply give $\zeta = 10^{-17}$ at $r > 3$ AU and $\zeta = 10^{-18}$ at $r < 3$ AU. The higher value corresponds to ionization by cosmic rays and X-rays, while the lower value corresponds to ionization by radionuclides. The boundary $r = 3$ AU is chosen to approximate the full solution to $\zeta(r, z)$ including these ionizing sources (see Figure 2(a) of O09).

Figure 17 illustrates how the MMSN model is mapped in the $h-f_D$ plane. The thick solid line in the figure shows the radial profiles of $f_D$ and $h$ for $\epsilon = 0.1$ and $a_0 = 0.1 \mu\text{m}$. This line moves upward in the figure as $a_0$ is increased, because $f_D$ and $h$ are related as

$$f_D = 8.4 \times 10^{-3} \left( \frac{a_0}{0.1 \mu\text{m}} \right)^{17/7} \left( \frac{\zeta}{10^{-17} \text{ s}^{-1}} \right)^{-6/7}h^{6/7}$$

(this can be directly shown from Equations (59) and (61)) and hence $f_D$ increases with $a_0$ for fixed $h$.

Let us see the outcome of fractal dust growth in different locations of the disk using the freezeout condition (Equation (57)). Since the condition depends on the three parameters $(f_D, f_E, h)$, the boundary between the growth and freezeout regions is a two-dimensional surface in the three-dimensional space. However, it will be useful to represent the boundary as a single curve in the $h$-$f_D$ plane by relating $f_E$ to either $f_D$ or $h$. Below, we use the relation $f_E = 1.1(a_0/0.1 \mu\text{m})^{11/6} f_D^{-1/6}$ obtained from Equations (59) and (60).

The thick dashed curve in Figure 17 shows below which the freezeout condition holds for $a_0 = 0.1 \mu\text{m}$ and $\epsilon = 0.1$. For this case, we see that the freezeout region covers 1–100 AU from the central star. This means that the electrostatic barrier inhibits fractal dust growth except in an inner region of $r \lesssim 1$ AU and a very outer region of $r \gtrsim 100$ AU. For comparison, we also show the line $(\mathcal{E}_E/\mathcal{E}_K)_{\text{max}} = 3$ with the thin solid curve (we again use the above relation between $f_E$ and $f_D$). This line roughly corresponds to the boundary between the growth/ freezeout regions predicted by the monodisperse theory (see Equation (47)). Comparing this line with the thick dashed curve, we see that the central region of $r \lesssim 1$ AU would also be included in the freezeout region if the bimodal growth mode as seen in Section 4 were not absent. From this fact, we can expect that the bimodal growth is particularly important for dust evolution at small heliocentric distances. It should be noted, however, that all of these results are dependent on the adopted disk model (e.g., laminar disk) and parameters (e.g., $a_0$). We will defer further investigation to Paper II.
5.2. Effect of Charge Dispersion

Up to here, we have assumed that all aggregates with the same radius have an equal charge \(Q_a\). In reality, the charge distribution has a nonzero variance, and hence aggregates can have a negative charge smaller than the mean value. Here, we show that the charge dispersion hardly affects the emergence of the total freezeout.

As shown in \(O09\), the charge distribution for aggregates of size \(a\) is well approximated by a Gaussian distribution with variance (see Equation (24) of \(O09\))

\[
\langle \delta Q^2 \rangle_a = \frac{1 + \Psi}{2 + \Psi} \alpha k_B T.
\]

(63)

In principle, it is possible to fully take this effect into account by averaging the collision kernel \(K\) over all \(Q_1\) and \(Q_2\). However, the average cannot be written in a simple analytic form. For this reason, we simply estimate the effect of the charge dispersion as follows. Clearly, the effect of the charge dispersion is significant only if \(\langle \delta Q^2 \rangle_a\) is much larger than \(\langle Q_a \rangle^2\). Using Equations (2), (15), and (63), the ratio of \(\langle \delta Q^2 \rangle_a / \langle Q_a \rangle^2\) can be written as

\[
\frac{\langle \delta Q^2 \rangle_a}{\langle Q_a \rangle^2} = \frac{1 + \Psi}{2(\langle \delta E \rangle + (2 + \Psi)}
\]

(64)

where \(\langle \delta E \rangle\) is the electrostatic energy for \(Q_1 = Q_2 = \langle Q_a \rangle\). Since \(1/2 \leq \langle 1 + \Psi \rangle / (2 + \Psi) \leq 1\) for all \(\Psi\), we find that the ratio \(\langle \delta Q^2 \rangle_a / \langle Q_a \rangle^2\) is of an order of \(\langle \delta E \rangle^{-1}\). We also find that \(\langle \delta Q^2 \rangle_a / \langle Q_a \rangle^2\) decreases as dust grows because \(\langle \delta E \rangle\) increases with \(N\).

Using Equation (64), let us consider whether the freezeout criterion (Equation (57)) is affected by the presence of the charge dispersion. With the charge dispersion ignored, the freezeout criterion is given by \(\langle \delta E \rangle(N_D) \gtrsim 6\). If this condition holds, we find from Equation (64) that \(\delta Q^2_a(N_D) \lesssim 0.08 \langle Q_a \rangle^2 (N_D)^2 (1 + \Psi) / (2 + \Psi) \lesssim 0.08 \langle Q_a \rangle^2(N_D)^2\). This means that the “true” value of \(\langle \delta E \rangle(N_D)\) (i.e., the value with the charge dispersion taken into account) is not much different from the “approximate” value \(\langle \delta E \rangle(N_D)\) as long as \(\langle \delta E \rangle(N_D) \gtrsim 6\). Hence, the charge dispersion hardly affects the emergence of the total freezeout.

5.3. Dependence on the Velocity Dispersion

In this study, we have assumed that the velocity dispersion is thermal (see our probability distribution function, Equation (8)). This assumption neglects any fluctuation in the drift acceleration \(g\). This will be reasonable if \(g\) is caused by stellar gravity \((g = \Omega_K^2 \zeta)\). By contrast, the validity of this approximation is unclear if \(g\) is driven by turbulence \((g \approx u_{\nu}/T_0)\). For example, recent MHD simulations by Carballido et al. (2008) suggest that \(g\) may fluctuate by 10% in MRI-driven turbulence. To check the robustness of our conclusion, we examine how the outcome of dust growth depends on the choice of the velocity dispersion.

Here, we consider the cases where the fluctuation in the differential drift velocity is as large as the mean value. We mimic this situation by replacing \(k_B T\) in Equation (8) by \(k_B T + M_D(\Delta u_D)^2\), where \(\Delta u_D\) is the mean relative velocity given by Equation (9). With the modified velocity distribution function, we carried out simulations for four sets of parameters as in Section 4.2. Figure 18 compares the evolution of \(\langle N \rangle\) and \(\langle N \rangle_m\) obtained here with that in Section 4.2 (Figure 14). We find no significant difference between the two results. This should be the case since the freezeout occurs when Brownian motion dominates over the differential drift (i.e., \(k_B T \gg M_D(\Delta u_D)^2\); see Section 4). Detailed inspection shows that the average masses grow slightly faster when the dispersion is added to the differential drift, but this is clearly a minor effect. Hence, we conclude that fluctuation in the differential drift velocity hardly affects the outcome of the dust growth.

5.4. Validity of the Fractal Growth Model

So far, we have assumed that dust grows into porous (fractal) aggregates. This assumption is true only when the impact energy is so low that compaction of aggregates upon collision is negligible. Here, we show that the collisional compaction is actually negligible when we consider the freezeout of dust growth.

It has been shown by Dominik & Tielens (1997) that the collisional compaction becomes effective when the impact energy exceeds \(E_{\text{roll}}\), where

\[
E_{\text{roll}} = 3\pi^2 \gamma a_0 \xi_{\text{crit}}
\]

(65)

is the energy needed for a monomer to roll on another monomer in contact by 90°. \(\gamma\) is the surface energy per unit area and is estimated as 25 erg cm\(^{-2}\) for rocky monomers and somewhat higher for icy monomers. \(\xi_{\text{crit}}\) is the critical rolling displacement for inelastic rolling and is theoretically constrained as \(> 2\ \text{Å}\) (Dominik & Tielens 1995).

As seen in the previous section, the total freezeout occurs when Brownian motion dominates aggregate compaction. Hence, the relative kinetic energy between frozen aggregates is equal to the thermal energy \(\sim k_B T\). Assuming \(T \sim 100\ \text{K}\), the thermal energy is \(10^{-14}\ \text{erg}\), which is many orders of magnitude lower than \(E_{\text{roll}}\). Therefore, collisional compaction is negligible whenever the total freezeout occurs.

Of course, the compaction is no longer negligible when the electrostatic barrier is overcome since the drift energy increases with aggregate mass and finally exceeds \(E_{\text{roll}}\). Investigation of dust growth after the fractal growth stage is beyond the scope of this study.
5.5. On the Role of Porosity Evolution

As shown in the previous subsection, it is valid to assume the fractal dust growth whenever we focus on the freezeout of dust growth. However, it has been still unclear whether the freezeout occurs even without the porosity evolution. Indeed, in previous studies on dust coagulation, it is common to ignore the porosity evolution and model aggregates as spheres of a fixed internal density (e.g., Weidenschilling 1977; Nakagawa et al. 1981; Tanaka et al. 2005; Brauer et al. 2008). To fully understand the robustness of the freezeout, we will discuss how the growth outcome changes if we adopt the compact aggregate model.

5.5.1. Drift and Electrostatic Energies for Compact Dust Particles

It is straightforward to write down the dimensionless energies \( E_D \) and \( E_E \) for the compact model. Since \( R = N^{1/3} \) and \( A = N^{2/3} \) for compact particles, Equations (26) and (27) are now replaced by

\[
E_D = f_D \frac{N_1 N_2}{N_1 + N_2} \left| \frac{N_1}{A_1} - \frac{N_2}{A_2} \right|^2 = f_D \frac{N_1 N_2}{N_1 + N_2} \left( N_1^{1/3} - N_2^{1/3} \right)^2
\]

and

\[
E_E = f_E \left( \frac{\Psi}{\Psi_\infty} \right)^2 \frac{R_1 R_2}{R_1 + R_2} = f_E \left( \frac{\Psi}{\Psi_\infty} \right)^2 \frac{(N_1 N_2)^{1/3}}{N_1^{1/3} + N_2^{1/3}},
\]

respectively. Note that \( \epsilon \) identically vanishes here by the definition of the compact dust model.

5.5.2. Simulations

Using Equations (66) and (67) instead of Equations (26) and (27), we have carried out simulations for several sets of \((f_D, f_E, h, \Psi_\infty)\). Figure 19 shows the results for the uncharged case \((h = 0)\) and three charged cases \((h = 10^{-2.5}, 10^{-4}, 10^{-5.5})\) with fixed \((f_D, f_E, \Psi_\infty) = (10^{-5}, 10, 10^{0.5})\). Note that the values of \((f_D, f_E, \Psi_\infty)\) are the same as those for the examples shown in Sections 4.1 and 4.2.

Without charging, the outcome of dust growth is qualitatively similar to that for the porous model (see the upper panel of Figure 12). Namely, we see power-law growth at early times \((T \lesssim 10^3)\) and exponential growth at later times \((T \gtrsim 10^3)\). One important difference is that the exponential growth begins at a lower mass \(N\) than in the porous case. As already mentioned in Section 3, the exponential growth is an indication that the differential drift takes over Brownian motion in the relative velocity between particles. In the porous model, the drift velocity of aggregates increases only slowly with mass, because the fractal dimension is close to 2 and hence the mass-to-area ratio \(N/A\) is nearly insensitive to \(N\). In the compact case, by contrast, the drift velocity increases with \(N\) \((\Delta u_D \propto N/A \propto N^{1/3})\). For this reason, the drift motion takes over Brownian motion \((\Delta u \propto N^{-1/2})\) at lower \(N\) than in the porous case.

The difference mentioned above consequently influences the outcome of dust growth with charging (the gray curves in Figure 19). We see that the total freezeout does not occur at \(h = 10^{-4}\) as it does in the porous case. This is because of the faster increase in the differential drift velocity mentioned above. In fact, the electrostatic energy also increases faster than in the compact case because of the faster decrease in the total projected area \(A_{\text{tot}}\) and capacitance \(C_{\text{tot}}\). However, this effect is small compared to the faster increase in the kinetic energy.

Therefore, we can say that the compact dust growth is resistive to the freezeout. Note that the compact growth is not free from the occurrence of the freezeout; in fact, we observe the freezeout for a higher-\(h\) case, \(h = 10^{-2.5}\).

We see that the mass distribution for \(h = 10^{-4}\) splits into two peaks. However, the evolution is qualitatively different from what we call bimodal growth in the porous case. The difference is that the low-mass peak gets continuously depleted as the high-mass peak grows toward higher \(N\). This occurs because the high-mass particles acquire arbitrarily high drift velocities as they grow. For the porous dust model, we have seen that the impact energy for highly unequal-sized collisions, \(E_{K,12}\), is nearly independent of the mass \(N_1\) of the heavier particle (see Section 4.2). In the compact model, by contrast, the impact energy is approximately given by \(E_{K,12} \approx 1 + f_D N_1 N_2^{2/3}\) (which directly follows from Equation (66) with \(N_1 \gg N_2\)), and this increases with \(N_1\). However, the electrostatic energy \(E_{E,12} \approx f_E (\Psi/\Psi_\infty)^2 R_2\) is independent of \(N_1\) as is in the porous case. Hence, we find that a high-mass particle with sufficiently large \(N_1\) can capture smaller particles.8

8 Strictly speaking, the decrease in the number of low-mass particles leads to the increase in \(\Psi\) (see Section 4.2), and hence proceeds in a way that \(E_{E,12}\) balances with \(E_{K,12}\) until \(\Psi\) reaches \(\Psi_\infty\).
Let us examine whether the condition for the freezeout is well described by the value of $\mathcal{E}_D(N_D)$ as is for the porous cases. The black dashed curve in Figure 20 shows the line where $\mathcal{E}_D(N_D)$ for the compact model is equal to 6. For comparison, the line $\mathcal{E}_D(N_D) = 6$ for the porous case (i.e., the dashed curve in the left panel of Figure 16) is also shown by the gray dashed curve. We find that the black line successfully explains the boundary between the freezeout and unimodal growth regions. Hence, we conclude that the freezeout criterion for the compact model is again given by Equation (57) if only we use Equation (70) for $\mathcal{E}_D(N_D)$.

To summarize this subsection, we have investigated how the growth outcome changes if one adopts a compact dust model. We confirmed that the total freezeout does occur even in the compact dust growth. This means that a fractal dust model is not a prerequisite for the emergence of the freezeout. However, this does not mean that the porosity evolution is negligible when we analyze the effect of the electrostatic barrier against dust growth. As shown above, the compact model makes dust growth more resistive to the freezeout because the differential drift takes over Brownian motion at a lower mass. Therefore, the porosity evolution must be properly taken into account in order not to overlook the significance of the electrostatic barrier.

6. SUMMARY

In this paper, we have investigated how the charging of dust affects its coagulation in weakly ionized protoplanetary disks. In particular, we have focused on the effect of the dust size distribution, which was ignored in the previous work (O09). We have used the porous (fractal) aggregate model recently proposed by OTS09 to properly take into account the porosity evolution of aggregates.

To clarify the role of the size distribution, we have divided our analysis into two steps. As the first step, in Section 3, we have presented a general analysis on the coagulation of charged aggregates under the monodisperse growth approximation. The monodisperse approximation allows us to define several useful quantities, such as the maximum energy ratio ($\mathcal{E}_K/\mathcal{E}_E$)max, the drift mass $N_D$, and the freezeout mass $N_F$. We have shown that, if the maximum energy ratio ($\mathcal{E}_K/\mathcal{E}_E$)max is larger than unity, the monodisperse growth stalls (or “freezes out”) at mass $N \approx N_F$, as was predicted by O09.

As the second step, in Section 4, we have calculated dust coagulation using the extended Smoluchowski method (OTS09) to examine how the outcome changes when the size dispersion is allowed to freely evolve. We find that, under certain conditions, the electrostatic repulsion leads to bimodal growth, rather than total freezeout. This bimodal growth is characterized by a large number of “frozen” aggregates and a small number of “unfrozen” aggregates, the former controlling the charge state of the system and the latter growing increasingly larger, carrying a major part of the system mass.

Based on the results of our numerical simulations, we have obtained a set of simple criteria that allows us to predict how the size distribution evolves for given conditions (Section 4.3; Table 2). These read as follows.

1. If $\mathcal{E}_E(N_D) \gtrsim 6$, all aggregates stops growing before the systematic drift dominates their relative velocities (“total freezeout”). The outcome is a nearly monodisperse distribution of frozen aggregates with typical mass $\approx N_F$.

2. If $\mathcal{E}_E(N_D) \lesssim 6$ and $\Psi \lesssim \Psi_\infty/4$, a large number of aggregates stop growing, but a major part of dust mass
within the system is carried by a small number of ever-growing aggregates (“bimodal growth”).

3. If $E(N_0) \lesssim 6$ and $\Psi_s \gtrsim \Psi_\infty/4$, all aggregates continue growing with a single-peaked size distribution (“unimodal growth”).

The second case includes situations where aggregates cannot continue growing in the monodisperse growth model. Thus, the size distribution is an important ingredient for the growth of dust aggregates beyond the electrostatic barrier.

We emphasize again that our analysis assumed fractal evolution of dust aggregates. This assumption is valid only when the collision energy is so small that collisional compaction is negligible (Dominik & Tielens 1997; Suyama et al. 2008). We have proven that the collisional compaction is indeed negligible as long as the total freezeout is concerned since the freeze-out always occurs when Brownian motion dominates aggregate collision (Section 5.4). It should be noted that most theoretical studies on dust coagulation (e.g., Nakagawa et al. 1981; Tanaka et al. 2005; Brauer et al. 2008) have ignored the porosity evolution and modeled aggregates as compact spheres. However, we have found that such simplification leads to understimation of the electrostatic barrier because compact spheres are frictionally less coupled to the gas and hence have higher drift velocities than porous aggregates of the same mass (Section 5.5). Therefore, the porosity evolution must be properly taken into account when considering the electrostatic barrier against dust growth in protoplanetary disks.

In Paper II, we apply our growth criteria to particular protoplanetary disk models to investigate the effect of the electrostatic barrier in the early stage of planet formation.

The authors thank the referee, Chris Ormel, for the many comments that greatly helped improve the manuscript. S.O. is supported by Grants-in-Aid for JSPS Fellows (22 · 7006) from MEXT of Japan.

**APPENDIX**

**NUMERICAL ESTIMATION OF THE AREA DISPERSION**

Let us consider two groups of porous aggregates each of which is characterized by aggregate mass $N_j (j = 1, 2)$. In either group, aggregates have different values of the projected area $A_j$. Therefore, the projected area, or the mass-to-area ratio $B_j = N_j / A_j$, of an aggregate randomly chosen from the $j$th group can be regarded as a stochastic variable. The average of the quantity $|B_1 - B_2|^2$ over all possible pairs is given by

$$
|B_1 - B_2|^2 = \langle B(N_1) - B(N_2) \rangle^2 + \sum_{j=1,2} \bar{\delta B}^2(N_j)
$$

where $\bar{B}(N_j)$ and $\bar{\delta B}^2(N_j)$ are the statistical average and variance of $B$ for aggregates of the $j$th group, and $\epsilon(N) \equiv \bar{\delta B}^2(N) / \bar{B}(N)$. Note that we have assumed that $B_1$ and $B_2$ are uncorrelated, i.e., $\bar{B}_1 \bar{B}_2 = \bar{B}(N_1) \bar{B}(N_2)$. Equation (A1) reduces to Equation (23) if $\epsilon(N)$ is independent of $N$. In this appendix, we estimate $\epsilon(N)$ using numerically created BCCA clusters.

We have performed 100 BCCA simulations and obtained the relation between $A$ and $N$ for each run. Since the projected area of an aggregate generally depends on the choice of the projection angle, we determined it as the average over 15 randomly chosen orientations. Figure 21 shows the mass-to-area ratio $B$ versus monomer number $N$ for 20 samples as well as the average $B$ over 100 samples. The area formula of Minato et al. (2006), Equation (21), is also plotted to show that $\bar{B}$ is consistent with the finding of Minato et al. (2006).

Figure 22 shows the ratio $\epsilon(N)$ obtained from 100 samples. For $10 \lesssim N \lesssim 10^6$, $\epsilon(N)$ is of an order of $10^{-1}$ and increases very slowly with $N$. Therefore, $\epsilon(N)$ can be well approximated as a constant $10^{-1}$. To check the convergence, we compute $\epsilon(N)$ using 50 of the samples. The small difference between the two curves means that the statistical error due to the finite number of samples is negligible.

Figure 22 implies that $\epsilon(N)$ may be considerably larger than $10^{-1}$ for $N \gg 10^6$. However, it should be noted that the above clusters have been formed through collisions between identical clusters. In reality, an aggregate in an ensemble collides with aggregates of various sizes. The most probable are collisions between aggregates of very different $B$, since the collision probability is proportional to $|B_1 - B_2|$. This effect generally causes the decrease in $\bar{\delta B}^2$ and hence the decrease in $\epsilon$. Therefore, the value of $\epsilon$ estimated here should be regarded as the upper limit of the actual values.

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