NUMERICAL MODELING OF THE COAGULATION AND POROSITY EVOLUTION OF DUST AGGREGATES

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1. INTRODUCTION

Porosity evolution of dust aggregates is crucial in understanding dust evolution in protoplanetary disks. In this study, we present useful tools to study the coagulation and porosity evolution of dust aggregates. First, we present a new numerical method for simulating dust coagulation and porosity evolution as an extension of the conventional Smoluchowski equation. This method follows the evolution of the mean porosity for each aggregate mass simultaneously with the evolution of the mass distribution function. This method reproduces the results of previous Monte Carlo simulations with much less computational expense. Second, we propose a new collision model for porous dust aggregates on the basis of our $N$-body experiments on aggregate collisions. As the first step, we focus on “hit-and-stick” collisions, which involve neither compression nor fragmentation of aggregates. We first obtain empirical data on porosity changes between the classical limits of ballistic cluster–cluster and particle–cluster aggregation. Using the data, we construct a recipe for the porosity change due to general hit-and-stick collisions as well as formulae for the aerodynamical and collisional cross sections. Our collision model is thus more realistic than a previous model of Ormel et al. based on the classical aggregation limits only. Simple coagulation simulations using the extended Smoluchowski method show that our collision model explains the fractal dimensions of porous aggregates observed in a full $N$-body simulation and a laboratory experiment. By contrast, similar simulations using the collision model of Ormel et al. result in much less porous aggregates, meaning that this model underestimates the porosity increase upon unequal-sized collisions. Besides, we discover that aggregates at the high-mass end of the distribution can have a considerably small aerodynamical cross section per unit mass compared with aggregates of lower masses. This occurs when aggregates drift under uniform acceleration (e.g., gravity) and their collision is induced by the difference in their terminal velocities. We point out an important implication of this discovery for dust growth in protoplanetary disks.

Key words: dust, extinction – planetary systems: formation – planetary systems: protoplanetary disks

ABSTRACT

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1. INTRODUCTION

It is a widely accepted idea that the first step of planet formation in protoplanetary disks involves the collisional growth of submicron/micron dust grains into macroscopic aggregates. A standard scenario is that dust grains coagulate by mutual sticking, gradually settle toward the midplane of the disk, and form a dense dust layer (e.g., Weidenschilling & Cuzzi 1993). It is still an open issue whether subsequent planetesimal formation is achieved by the gravitational instability of the layer (Safronov 1969; Goldreich & Ward 1973; Sekiya 1998; Youdin & Shu 2002) or by the direct collisional growth of the aggregates (Weidenschilling & Cuzzi 1993; Stepiński & Valageas 1997; Brauer et al. 2008). To address this issue, further understanding on earlier evolutionary stages is needed.

Most of the previous studies have simplified dust aggregates as compact, nonporous spheres. However, both numerical and laboratory experiments have revealed that aggregates are not at all compact, but have an open, fluffy structure (for a review, see Blum 2004; Dominik et al. 2007). This is particularly true for aggregates formed at an early growth stage where the collisional velocity is so low that collisional compression is negligible. It has been observed in $N$-body (Kempf et al. 1999) as well as experimental (Wurm & Blum 1998; Blum et al. 1998, 2000) studies that the outcome is an ensemble of fractal aggregates with the fractal dimension of $D < 2$. This fractal growth lasts until the impact energy becomes high enough to cause collisional compaction (Suyama et al. 2008). The porosity change due to compressive as well as destructive collisions are also studied by some authors (e.g., Wada et al. 2007, 2008, 2009; Suyama et al. 2008; Paszun & Dominik 2009) using $N$-body simulations including monomer surface interactions (Dominik & Tielens 1997).

There are several strong reasons why the porosity evolution of aggregates is important in studying dust evolution in protoplanetary disks. These include the following.

1. The porosity affects the aerodynamical property of aggregates. In a gas disk, the motion of a small aggregate is controlled by the friction force from the ambient gas. The friction coefficient can vary by many orders of magnitude depending on whether the aggregate is compact or fluffy. For example, a fractal ($D < 2$) aggregate made of one thousand grains receives a friction force an order of magnitude stronger than a compact aggregate of the same mass. This difference is significant when one considers the formation of sedimentary dust layer on the disk midplane.

2. The porosity even affects the turbulence of protoplanetary disks. Magnetorotational instability (MRI; Balbus & Hawley 1991), which is recognized as the most likely mechanism driving disk turbulence, operates only in a region where the ionization degree is sufficiently high (Gammie 1996). The ionization degree strongly depends on the surface area of dust aggregates, since the recombination of ionized gases efficiently takes place on dust surfaces. Again, a fractal ($D < 2$) aggregate made of one thousand grains...
absorbs ionized gases an order magnitude more efficiently than a compact grain of the same mass. For this reason, compact dust growth tends to make the gas environment turbulent (Sano et al. 2000), while fractal dust growth tends to keep the environment laminar (Okuzumi 2009). This difference is critical to the evolution of dust itself, since the turbulence causes the diffusion and collisional fragmentation of aggregates (Brauer et al. 2008; Johansen et al. 2008).

3. The fractal nature of aggregates matters when we try to interpret observed emission spectra of protoplanetary disks. For example, the 10 μm spectral feature characteristic of submicron silicate grains quickly vanishes in compact aggregation, but only slowly in fractal ($D \sim 2$) aggregation (Min et al. 2006). This means that the conventional compact dust model generally underestimates the degree of dust growth in the observed objects.

Thus, the consistent modeling of the growth and porosity evolution of dust aggregates is needed to better understand and predict dust evolution in protoplanetary disks.

Theoretically, however, the consistent modeling is not an easy task. First of all, we must consider the evolution of aggregates in the two-dimensional (2D) parameter space of mass and porosity. However, such 2D calculation is generally much more elaborate than one-dimensional (1D; i.e., mass only) one. Furthermore, such calculation requires a reliable collision model for porous aggregates. Here, a “collision model” refers to a set of (1) the definition of the “porosity” or “volume” of an aggregate, (2) a recipe that determines the porosity change due to collisions, and (3) formulae for collisional and aerodynamical cross sections that determine the collision rate of porous aggregate pairs. To obtain a reliable collision model, one needs a sufficient amount of empirical data on aggregate collisions.

Because of the above theoretical difficulty, there are only a few studies addressing the coagulation of porous dust aggregates in the literature. A 2D simulation on porous dust growth was first done by Ossenkopf (1993) in the context of dust extinction in molecular clouds. He used a collision model based on the $N$-body simulations of the ballistic cluster–cluster and particle–cluster aggregation (BCCA and BPCA; Meakin 1991). Ormel et al. (2007; hereafter, OST07) have presented a Monte Carlo method for studying porosity evolution of dust aggregates in protoplanetary disks. In this method, porous aggregates are represented by the same number of computational particles with mass and porosity; and the collisions among the particles are successively calculated using random numbers. The change in porosity on each individual collision is determined from a recipe based on previous $N$-body experiments on aggregate collisions (Ossenkopf 1993; Dominik & Tielens 1997). The Monte Carlo approach has been further developed independently by Ormel & Spaans (2008) and Zsom & Dullemond (2008) to achieve a high dynamical range in the parameter space. The compression/fragmentation model of OST07 has been recently revised by Ormel et al. (2009) on the basis of numerical experiments on low-mass aggregate collisions (Paszun & Dominik 2009).

In this study, we provide new theoretical tools useful for studying the collisional evolution of porous dust aggregates. First, we present a new numerical method to solve the growth and porosity evolution of aggregates. This method is an extension of the conventional Smoluchowski method, a method commonly used for 1D simulations of dust aggregates (e.g., Tanaka et al. 2005; Dullemond & Dominik 2005; Brauer et al. 2008). The core of our new method is the approximation that the porosity distribution is narrow for each aggregate mass.

With this approximation, we derive a closed set of moment equations of the 2D Smoluchowski equation for the mass distribution function and the averaged mass–porosity relation. These equations are formally similar to the conventional 1D Smoluchowski equation, and makes it possible to adopt well-established algorithms for 1D problems. We confirm that this approach indeed reproduces the results of the Monte Carlo simulations by OST07 with much less computational effort. Thus, our method will be particularly useful for adding the porosity evolution to global simulations including radial drift (e.g., Brauer et al. 2008) or coupled simulations involving hydrodynamical calculation (e.g., Johansen et al. 2008). Second, we provide a new collision model based on our $N$-body experiments for various types of aggregate collisions. As the first step of the modeling, we focus on “hit-and-stick” collision, i.e., low-velocity collision involving neither compression nor fragmentation. In a typical protoplanetary disk, the hit-and-stick picture well represents the growth of dust aggregates up to several centimeters (Suyama et al. 2008). In contrast to previous studies, we use empirical data on the porosity evolution between the BCCA and BPCA limits. We will see that the numerical simulations of porosity evolution using our collision model well agree with the results of previous full $N$-body and laboratory experiments. Extension of our model to compressive and destructive collisions will be made in the future work.

This paper is organized as follows. In Section 2, we describe our extended Smoluchowski method and its numerical implementation. In Section 3, we use this method to try to reproduce the results of the Monte Carlo simulations by OST07. In Section 4, we present a new porosity model as well as the results of our $N$-body simulations from which we construct the porosity increase recipe. In Section 5, we compare this collision model with that of OST07. Section 6 is devoted to the summary.

2. THE EXTENDED SMOLUCHOWSKI METHOD FOR POROUS DUST GROWTH

In this section, we describe a new method to solve the coagulation and porosity evolution of dust aggregates. A comparison between our method and the Monte Carlo method is made in Section 3.

2.1. The Multi-dimensional Smoluchowski Equation

We denote the internal structure of each aggregate by a set of parameters $\mathbf{I} = \{I^{1}, I^{2}, \ldots\}$. Conventional coagulation models adopted the mass $M$ of an aggregate as a unique parameter, i.e., $\mathbf{I} = \{M\}$. This study treats the volume $V$ as an additional parameter for porous aggregates. We assume that the internal structure of an aggregate created by a collision is uniquely determined by those of the collided ones. This means that the structure parameter of the new aggregate, $I_{1+2}$, is a function of those of the old ones, $I_{1}$ and $I_{2}$.

We denote the distribution function of aggregates by $f(\mathbf{I})$. The evolution of $f(\mathbf{I})$ is determined by the multi-dimensional Smoluchowski equation

$$\frac{\partial f(\mathbf{I})}{\partial t} = \frac{1}{2} \int d\mathbf{I}' d\mathbf{I}'' K(\mathbf{I}; \mathbf{I}') f(\mathbf{I}) f(\mathbf{I}'') \times \delta[I_{1+2}(\mathbf{I}; \mathbf{I}'') - I] - f(\mathbf{I}) \int d\mathbf{I}' K(\mathbf{I}; \mathbf{I}') f(\mathbf{I}') \tag{1}$$

where $K(\mathbf{I}_{1}; \mathbf{I}_{2}) = K(\mathbf{I}_{1}; \mathbf{I}_{1})$ is the collision kernel defined as the product of the collision cross section $\sigma_{\text{coll}}$ and the relative
speed $\Delta u$ of colliding pairs. The first and second terms in Equation (1) represent the “gain” and “loss” of aggregates with I due to collisions, respectively.

If I only contains $M$, Equation (1) reduces to the conventional, 1D Smoluchowski equation

$$\frac{\partial f(M)}{\partial t} = \frac{1}{2} \int_{0}^{\infty} dM' K(M'; M - M') f(M') f(M - M') - f(M) \int_{0}^{\infty} dM' K(M'; M') f(M'),$$

(2)

where we have used the mass conservation $M_{1+2}(M', M'') = M' + M''$. It is easy to check that Equation (2) ensures the conservation of the total mass density $\rho_d = \int M f(M) dM$.

Now we consider the 2D case, $I = (M, V)$. In this case, Equation (1) is written as

$$\frac{\partial f_{M,V}}{\partial t} = \frac{1}{2} \int_{0}^{M} dM' \int dV' dV'' K_{M,M',V',V''}^{M',V,V} f_{M',V'} f_{M-M',V'},$$

(3)

$$\times \delta[(V_{1+2}^{M',V'} - V)],$$

$$- f_{M,V} \int dM' dV' K_{M,M',V',V''}^{M',V,V} f_{M',V'},$$

where $f_{M,V} \equiv f(M, V)$, $K_{M,M',V',V''}^{M',V,V} \equiv K(M', V'; M'', V'')$, and $(V_{1+2}^{M',V'} - V) = V_{1+2}(M', V'; M'', V'')$. Again, one can easily check that Equation (3) ensures the conservation of the total mass density $\rho_d = \int M f(M, V) dMdV$ for arbitrary $V_{1+2}$.

2.2. The Volume-averaging Approximation

In principle, the 2D Smoluchowski Equation (3) can be solved once $K$ and $V_{1+2}$ are given. In practice, however, direct numerical integration of Equation (3) requires a huge computational expense. To see this, let us consider that we try to solve Equation (3) by dividing each parameter dimension with $N$ fixed bins. At each step, we have to calculate collision events over all pairs of the bins. For a $D$-dimensional problems, the number of the fixed bins is $N^D$, so the total number of the collision pairs is approximately $N^{2D}$. Thus, we see that a 2D calculation of the Smoluchowski equation is approximately $N^2$ times heavier than a 1D one. Of course, one is free to take very small $N$, but then it would result in a very poor resolution of $f(M, V)$. For a practical use, some prescription is clearly needed to manage both a reasonably small expense and reasonably good accuracy. One option may be to use fewer bins and instead continuously adjust them so that they span a parameter region with large $f(M, V)$. This approach appears to be efficient only if the adjustment requires only a few calculations. Another option is to adopt a direct Monte Carlo method, as done by OST07 and Zsom & Dullemond (2008). Monte Carlo methods are effectively similar to the moving bin method since the Monte Carlo particles are continuously redistributed in the 2D space.

Now we propose a new method. A basic strategy of this method is to take up following details of the volume distribution and to only follow its average for each mass. This enables us to calculate the porosity evolution with only $O(N^2)$ calculations at each time step as is for 1D problems.

For a rigorous formulation, we introduce the moments of the 2D distribution function

$$n(M) \equiv \int f(M, V) dV,$$

(4)

$$\overline{V}(M) \equiv \frac{1}{n(M)} \int V f(M, V) dV,$$

(5)

where $n(M)$ and $\overline{V}(M)$ denote the number density and mean volume of aggregates with mass $M$, respectively. The evolution of these quantities is described by the moment equations of the 2D Smoluchowski equation, Equation (3). Taking the zeroth- and first-order moments of Equation (3) with respect to $V$, we obtain

$$\frac{\partial n(M)}{\partial t} = \frac{1}{2} \int_{0}^{M} dM' \overline{K}(M'; M - M') n(M') n(M - M')$$

$$- n(M) \int_{0}^{\infty} dM' \overline{K}(M; M') n(M'),$$

(6)

and

$$\frac{\partial [\overline{V}(M) n(M)]}{\partial t} = \frac{1}{2} \int_{0}^{M} dM' \overline{K}(M'; M - M')$$

$$\times n(M') n(M - M')$$

$$- n(M) \int_{0}^{\infty} dM' \overline{V}(M; M') n(M'),$$

(7)

where $\overline{K}$, $\overline{V}_{1+2}$, and $\overline{V} \overline{K}$ are the volume averages of $K$, $V_{1+2}$, and $V \overline{K}$ defined by

$$\overline{K}(M'; V') \equiv \int dV' dV'' K_{M,M',V',V''}^{M',V,V} f_{M',V'} f_{M-M',V'},$$

(8)

$$\overline{V}_{1+2}(M'; V') \equiv \int dV' dV'' (V_{1+2}^{M',V'}) K_{M,M',V',V''}^{M',V,V}$$

$$\times f_{M',V'} f_{M-M',V'},$$

(9)

$$\overline{V} \overline{K}(M; V') \equiv \int dV' \int dV'' V_{M,M',V',V''} f_{M',V'} f_{M-M',V'}/n(M) n(M'),$$

(10)

Note that the above volume-averaged quantities generally depend on higher order moments of $V$. To solve Equations (6) and (7) in a closed way, some additional assumption about the higher order moments is needed.

Now we try to close Equations (6) and (7) in terms of $n(M)$ and $\overline{V}(M)$ by making a simple assumption. The simplest one is that the volume distribution is so narrow that the volume moments higher than the first order can be ignored. This assumption is equivalent to supposing that the distribution function $f(M, V)$ is well approximated in the form

$$f(M, V) = n(M) \delta[V - \overline{V}(M)],$$

(11)

Using this assumption, the volume integral in Equations (8)–(10) can be performed for arbitrary $K$ to give

$$\overline{K}(M'; M'') = K(M', \overline{V}(M'); M'', \overline{V}(M'')),$$

(12)

$$\overline{V}_{1+2}(M'; M'') = V_{1+2}(M', \overline{V}(M'); M'', \overline{V}(M'')) \overline{K}(M'; M''),$$

(13)

and

$$\overline{V} \overline{K}(M; M') = \overline{V}(M) \overline{K}(M'; M'').$$

(14)
Substituting these into Equations (6) and (7), we obtain the closed forms of the moment equations
\[
\frac{\partial n(M)}{\partial t} = \frac{1}{2} \int_0^M dM' K_{M\to M'} n(M') n(M - M') - n(M) \int_0^\infty dM' K_{M'\to M'M} n(M'),
\]
and
\[
\frac{\partial (V(M)n(M))}{\partial t} = \frac{1}{2} \int_0^M dM' (V_{1+2})_{M\to M'} n(M') \times K_{M'\to M'M} n(M') n(M - M') - \nabla (V(M)n(M)) \int_0^\infty dM' K_{M'\to M'M} n(M').
\]
(15) and (16)

In this way, we have reduced the 2D Smoluchowski equation, Equation (3), to a closed set of two 1D Equations (15) and (16) just by imposing a simple approximation, Equation (11). We refer to this assumption as the volume-averaging approximation.

The set of Equations (15) and (16) has several advantages over the original full 2D Equation (3). First, since all the volume integrals has been already performed, Equations (15) and (16) only requires $O(N^2)$ calculations at each time step. Second, as explained in the following subsection, one can solve these equations in just the same way as one solves the conventional 1D Equation (2). The drawback is that we do not know in advance whether the approximation made by Equation (11) is reasonable or not for a coagulation problem to be solved. Nevertheless, we will see in Section 3 that this approximation is surprisingly successful in reproducing the results of previous full 2D calculations.

It is worth mentioning here that the above formulation can be extended to other aggregate parameters. For example, it is straightforward to derive equations like Equations (15) and (16) with the electric charge $Q$ as an additional parameter. This charge-averaging approximation will be particularly useful in a situation where aggregate collisions lead to charge separation between small and large aggregates. Recently, Muranushi (2009) has shown that, with a sufficiently high dust-to-gas ratio, the charge separation could occur for icy aggregates in protoplanetary disks. The charge separation is potentially important since it can lead to the lightning in the disks, which is a possible mechanism for chondrule formation (Desch & Cuzzi 2000). The charge-averaging approximation will offer a powerful tool for further investigation of this issue.

2.3. Numerical Implementation

Before proceeding to the numerical implementation of Equations (15) and (16), we briefly review how the 1D Smoluchowski equation, Equation (2), has been solved numerically. Let us rewrite Equation (2) as
\[
\frac{\partial (M f_M)}{\partial t} = \int_0^{M/2} dM' M_{1+2} K_{M',M'M} f_{M'} f_{M'} - \int_0^{\infty} dM' M K_{M',M'M} f_{M'} f_{M'},
\]
where $f_M = f(M)$, $K_{M',M} = K(M'; M')$, $M'' = M - M'$, and $M_{1+2} = M' + M'' = M$. This equation means that the mass density $M f_M$ increases by the collision between aggregates $M'$ and $M''(< M')$ at a rate $M_{1+2} K_{M',M'M} f_{M'} f_{M'}$, and decreases by the collision between $M$ and $M'$ at a rate $M K_{M',M'M} f_{M'} f_{M'}$. A numerical calculation of a 1D coagulation problem often employs Equation (17) instead of Equation (2), and regards $M f_M$ as a fundamental quantity to be evolved (e.g., Nakagawa et al. 1981; Tanaka et al. 2005). This formulation ensures the conservation of the total mass density $\rho = \int_0^{\infty} M f_M$ in an exact way.

Now we go back to the 2D case. Let us rewrite Equations (15) and (16) as
\[
\frac{\partial (M n_M)}{\partial t} = \int_0^{M/2} dM' M_{1+2} K_{M',M'M} f_{M'} f_{M'} - \int_0^{\infty} dM' M K_{M',M'M} f_{M'} f_{M'} n_{M,M'},
\]
and
\[
\frac{\partial (V n_M)}{\partial t} = \int_0^{M/2} dM' (V_{1+2})_{M',M'M} K_{M',M'M} f_{M'} f_{M'} n_{M,M'} - \int_0^{\infty} dM' V K_{M',M'M} f_{M'} f_{M'} n_{M,M'},
\]
respectively, where $n_M = n(M)$. Note that these equations are very similar to the 1D Equation (17). In fact, Equation (18)

reduces to Equation (17) just by rewriting $K_{M',M'M}$ as $K_{M',M'M'}$. Furthermore, Equations (18) and (19) are formally identical except that $M$ and $M_{1+2}$ in the former equation are replaced by $V$ and $V_{1+2}$ in the latter. Thus, we need not to prepare any special numerical scheme to solve Equations (18) and (19); we only need to adopt a scheme that has been developed to solve the conventional Equation (17).

In this study, we solve Equations (18) and (19) using a fixed-bin scheme (Nakagawa et al. 1981; Tanaka et al. 2005; Brauer et al. 2008). In this scheme, the mass space is divided into discrete bins and collision events are calculated among the bins. For monodisperse monomers with mass $m_0$, the mass regions $m_0 \leq M \leq N_{bd} m_0$ are divided into linearly spaced bins with representative mass $M_k = k m_0$ ($k = 1, 2, \ldots, N_{bd}$), and the regions $M > N_{bd} m_0$ are divided into logarithmically spaced bins with $M_k = 10^{k/k_{bd}} M_{k-1}$ ($k > N_{bd}$). For polydisperse monomers, the mass spaces are just divided logarithmically. In this study, we do not consider polydisperse monomers. As pointed out by Ohtsuki et al. (1990), the choice of $N_{bd}$ must be carefully done because a small value of $N_{bd}$ can cause artificial acceleration in coagulation at the high-mass distribution tail. Lee (2000) performed a couple of simulations with different $N_{bd}$ and found that the numerical solutions converge for $N_{bd} = 40$. In this study, we take $N_{bd} = 40$ or 80 (or equivalently, $M_{1+1}/M_k = 1.06$ or 1.03) depending on problems considered.

Transfer of mass and volume in the mass space are calculated in the following way. The number $Q_{ij}$ of collision events per unit time between two bins $i$ and $j$ ($j \geq i$) is written as $Q_{ij} = K_{ij} n_i n_j$ for $j > i$ and $Q_{ij} = (1/2) K_{ii} n_i^2$ for $j = i$. The total mass densities transferred from bins $i$ and $j$ in the events are $M_j Q_{ij}$ and $M_i Q_{ij}$, and the total volume densities transferred are $V_j Q_{ij}$ and $V_i Q_{ij}$, respectively. As a natural consequence of the logarithmic binning, the mass of the resulting aggregates, $M_{ij} = M_i + M_j$, does not necessarily coincide with any of the bin masses, and generally goes between $M_i$ and $M_{i+1}$ with some $\ell (\geq j)$. Therefore, we have to determine the mass
densities transferred to bins $\ell$ and $\ell + 1$ in some way. In this study, we adopt a prescription of Kovetz & Olund (1969), in which the mass densities transferred to bins $\ell$ and $\ell + 1$ are determined as $\varepsilon M_{ij} Q_{ij}$ and $(1-\varepsilon)M_{ij} Q_{ij}$, respectively, where $\varepsilon = (M_{\ell+1} - M_{ij})/(M_{\ell+1} - M_{ij})$. This prescription ensures the conservation of the total number and total mass of the resulting aggregates (see Appendix A.1 of Brauer et al. 2008). Similarly, the volume densities transferred to bins $\ell$ and $\ell + 1$ are determined as $\varepsilon V_{ij} Q_{ij}$ and $(1-\varepsilon)V_{ij} Q_{ij}$, where $V_{ij} = V_{i+2}(M_i, \overline{V}(M_i); M_j, \overline{V}(M_j))$. For $\ell = j$, we compute the gain and loss of the mass and volume densities in bin $j$ simultaneously, i.e., only compute the net gains $\varepsilon M_{ij} Q_{ij}$ and $(V_{ij} - \overline{V}(M_{ij}))Q_{ij}$. This simultaneous computation avoids systematically increasing errors in the densities due to the near cancellation of the gain and loss terms beyond the double precision (see Appendix B of Dullemond & Dominik 2005). Also, we adopt the “active” bin method (Lee2000; Tanaka et al. 2005) in which collisions are not allowed for mass bins with negligibly small mass/number densities. This method greatly reduces the computational expense because high-mass and low-mass bins are mostly empty in early and later evolutionary stages, respectively. Following Tanaka et al. (2005), we take the critical minimum mass density for each mass bin to be $10^{-25}$ times the total mass density, $\rho_d$, of the system. A test simulation by Tanaka et al. (2005) shows that this prescription hardly affects the evolution of the mass distribution function.

For time integration, we adopt the explicit, fourth-order Runge–Kutta method. The time step $\Delta t$ is continuously adjusted so that the fractional decrease in mass density at any bin does not exceed a constant parameter $\delta$ (typically between 0.01 and 0.1). Although we use the explicit integration scheme for simplicity, the use of an implicit scheme (e.g., Brauer et al. 2008) would further reduce the computational expense because high-mass and low-mass bins are mostly empty in early and later evolutionary stages, respectively. Following Tanaka et al. (2005), we take the critical minimum mass density for each mass bin to be $10^{-25}$ times the total mass density, $\rho_d$, of the system. A test simulation by Tanaka et al. (2005) shows that this prescription hardly affects the evolution of the mass distribution function.

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3. COMPARISON BETWEEN THE EXTENDED SMOLUCHOWSKI METHOD AND FULL 2D MONTE CARLO METHODS

To demonstrate the accuracy of our extended Smoluchowski method, we apply this method to try to reproduce the results of full 2D Monte Carlo simulations by OST07. This problem has been also solved by Zsom & Dullemond (2008) to compare their Monte Carlo method with that of OST07.

In Sections 3.1 and 3.2, we briefly summarize the collision model and the protoplanetary disk model assumed in the OST07 problem. In Section 3.3, we show the results of our calculation and compare them with those of OST07 and Zsom & Dullemond (2008).

3.1. The Collision Model of OST07

Here we summarize the porous aggregate model adopted by OST07. An aggregate is modeled as a cluster consisting of $N$ monodisperse dust grains (monomers) of mass $m_0$ and radius $a_0$. The porosity of an aggregates is represented by the "enlargement factor"

$$\psi \equiv \frac{V_A}{V_\star},$$

where $V_\star = NV_0$ is the compact volume, and

$$V_A = V_0 \left( \frac{A}{A_0} \right)^{3/2}$$

is the “volume” defined by the projected area $A$ of the aggregate. $V_0$ and $A_0$ are the volume and the geometric cross section of a monomer given by $V_0 = (4\pi/3)a_0^3$ and $A_0 = \pi a_0^2$, respectively.

Below, we refer to $V_A$ as the area-equivalent volume. A compact aggregate has $\psi = 1$, while a porous aggregate has $\psi > 1$. Each aggregate is thus characterized by its mass $M = Nm_0$ and enlargement factor $\psi$.

The enlargement factor after a collision, $\psi_{1+2} = \psi_{1+2}(M_1, \psi_1; M_2, \psi_2)$, is determined in two different ways depending on the value of the impact energy. The impact energy is defined by $E = (1/2)\dot{M}(\Delta u)^2$, where $\dot{M} = (M_1/M_2)/(M_1 + M_2)$ is the reduced mass and $\Delta u$ is the relative velocity. If $E$ is smaller than the critical restructuring energy $E_{\text{restr}}$, the collided aggregates just stick to each other without compression (“hit-and-stick” regime). If $E > E_{\text{restr}}$, the collision involves the compaction of the aggregates and another formula is applied for $\psi_{1+2}$ (compaction regime). The critical restructuring energy is set to the rolling energy $E_{\text{roll}}$ given by $E_{\text{roll}} = (\pi a_0/2)F_{\text{roll}}$, where $F_{\text{roll}}$ is the rolling-friction force. OST07 adopted $F_{\text{roll}} = 8.5 \times 10^{-7} (\gamma/14$ erg cm$^{-2}$) dyn as suggested by a laboratory experiment (Heim et al. 1999).

In the hit-and-stick regime, the formula for $\psi_{1+2}$ is given by (Equation (15) of OST07)

$$\psi_{1+2} = \frac{M_1 \psi_1 + M_2 \psi_2}{M_1 + M_2} \left( \frac{M_1 \psi_1 + M_2 \psi_2}{M_1 \psi_1} \right)^{3\text{CCA}/2-1} + \psi_{\text{add}},$$

(22)

where $\delta_{\text{CCA}} = 0.95$ and $\psi_{\text{add}}$ is an additional factor only relevant to BPCA-like collisions (see Equation (19) of OST07).

Rewriting Equation (22) in terms of $V_A$ instead of $\psi$, we obtain

$$V_{A,1+2} = V_{A,1} \left( \frac{V_{A,1} + V_{A,2}}{V_{A,1}} \right)^{3\text{CCA}/2} + \psi_{\text{add}}V_{A,1+2},$$

(23)

where $V_{A,1+2} = V_{A,1} + V_{A,2} = V_0(N_1 + N_2)$ is the “compact volume” (the volume occupied by the constituent monomers) of the newly formed aggregate. OST07 constructed the above formula so that it agrees with the N-body results of Ossenkopf (1993) in the BCCA and BPCA limits. However, as we show in Section 4.1, the above formula is invalid between the two limits. For $N_1 + N_2 \leq 40$, the enlargement factor $\psi_{1+2}$ is directly determined by the fitting formula of Ossenkopf (1993).

In the compaction regime, $\psi_{1+2}$ is given by

$$V_{A,1+2}(\psi_{1+2} - 1) = (1 - f_C)[V_A(\psi_1 - 1) + V_{A,2}(\psi_2 - 1)],$$

(24)

where $f_C = E/[(N_1 + N_2)E_{\text{roll}}]$. Using the relation $V_A = V_\star \psi$, we obtain the corresponding formula for $V_{A,1+2}$,

$$V_{A,1+2} = V_{A,1} + V_{A,2} - f_C(V_{A,1} + V_{A,2} - V_{A,1+2}).$$

(25)

OST07 constructed this formula by assuming that the relative decrease in the porous volume $V_A - V_\star = V_A(\psi - 1)$ scales linearly with $E$. However, Wada et al. (2008) have recently shown that this formula does not reproduce the results of N-body simulations.

The collisional cross section $\sigma_{\text{coll}}$ is given by $\sigma_{\text{coll}} = \pi(a_{A,1} + a_{A,2})^2$, where

$$a_A \equiv \sqrt{\frac{A}{\pi}} = a_0 \left( \frac{V_A}{V_0} \right)^{1/3},$$

(26)

is the area-equivalent radius, i.e., the radius defined by the projected area $A$. 

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and assumed rocky dust for $R$ and take the dust parameters as $\rho_g/\rho_d$ scheme are set to $N_{MSN}$ values. OST07 made some order of unity errors in calculating these $3$ Note that the values of $\alpha$ and $T$ are given by power laws $\Sigma \propto R^{-3/2}$ and $T \propto R^{-1/2}$, where $R$ is the distance from the central star. They considered two disk positions $R = 1$AU and 5AU, and assumed rocky dust for $R = 1$AU and icy dust for $R = 5$AU. In this study, we consider the case of $R = 1$AU, and take the dust parameters as $\rho_g/\rho_d = 240, \alpha_0 = 0.1 \mu m, \rho_0 = 3.0 g cm^{-3}$, and $\gamma = 25 erg cm^{-2}$. The strength of disk turbulence is parameterized by the so-called $\alpha$-parameter $\alpha_T$. OST07 considered three cases: $\alpha_T = 10^{-6}, 10^{-4},$ and $10^{-2}$. The vertical position is taken as one scale height above the midplane. The collision velocity is induced by Brownian motion and turbulence. An aggregate is removed from the population (or “rains out” to the midplane) if its stopping time $\tau$ exceeds the critical value $\tau_{rain} = \alpha_T/\Omega$, where $\Omega$ is the Kepler rotational frequency. The mass of the central star is taken as $1 M_{\odot}$, so that $\Omega$ is given by $\Omega = 2.0 \times 10^{-7}rad s^{-1}$ at $R = 1$AU. OST07 adopted $\rho_g = 8.5 \times 10^{-10} g cm^{-3}, c_r = 1.6 \times 10^5 cm s^{-1}, \rho_g/\rho_d = 240$, the dust material density $\rho_0 = 3.0 g cm^{-3}$, and the critical rolling energy $E_{roll} = 2.4 \times 10^{-9}$erg.

3.2. Protoplanetary Disk Model

OST07 adopted the minimum-mass solar nebula (MMSN) model (Hayashi 1981) in which the gas surface density $\Sigma_\infty$ and the temperature $T$ are given by power laws $\Sigma_\infty \propto R^{-3/2}$ and $T \propto R^{-1/2}$, where $R$ is the distance from the central star. They considered two disk positions $R = 1$AU and 5AU, and assumed rocky dust for $R = 1$AU and icy dust for $R = 5$AU. In this study, we consider the case of $R = 1$AU, and take the dust parameters as $\rho_g/\rho_d = 240, \alpha_0 = 0.1 \mu m, \rho_0 = 3.0 g cm^{-3}$, and $\gamma = 25 erg cm^{-2}$. The strength of disk turbulence is parameterized by the so-called $\alpha$-parameter $\alpha_T$. OST07 considered three cases: $\alpha_T = 10^{-6}, 10^{-4},$ and $10^{-2}$. The vertical position is taken as one scale height above the midplane. The collision velocity is induced by Brownian motion and turbulence. An aggregate is removed from the population (or “rains out” to the midplane) if its stopping time $\tau$ exceeds the critical value $\tau_{rain} = \alpha_T/\Omega$, where $\Omega$ is the Kepler rotational frequency. The mass of the central star is taken as $1 M_{\odot}$, so that $\Omega$ is given by $\Omega = 2.0 \times 10^{-7}rad s^{-1}$ at $R = 1$AU. OST07 adopted $\rho_g = 8.5 \times 10^{-10} g cm^{-3}, c_r = 1.6 \times 10^5 cm s^{-1}, \rho_g/\rho_d = 240$, the dust material density $\rho_0 = 3.0 g cm^{-3}$, and the critical rolling energy $E_{roll} = 2.4 \times 10^{-9}$erg.

3.3. Results and Comparison

Following OST07, we have performed simulations for four growth models: three porous ($\alpha_T = 10^{-6}, 10^{-4},$ and $10^{-2}$) and one compact ($\alpha_T = 10^{-4}$). We computed the evolution of $n(M)$ and $\Sigma_\infty(M)$ using Equations (18) and (19) with the numerical scheme described in Section 2.3. The control parameters of the scheme are set to $N_{bd} = 40$ and $\delta = 0.1$. We have confirmed the numerical result is insensitive to the values of $N_{bd}$ and $\delta$ as long as $N_{bd} \geq 40$ and $\delta \leq 0.1$. The volume $V_{A,1+2}$ of newly formed aggregates is calculated in accordance with the collision model of OST07.

Figure 1 shows the evolution of the mass distribution function for the porous, $\alpha_T = 10^{-4}$, model. This figure corresponds to Figure 10C in OST07. One can readily see that the evolution of our distribution function is qualitatively very similar to that of the OST07: nearly monodisperse growth due to Brownian motion for $t \lesssim 10^3$ yr, exponential growth driven by turbulence for $10^3 yr \lesssim t \lesssim 10^4$ yr, and “rain-out” with porous size $a_A \approx 2$ cm for $t \gtrsim 10^4$ yr. More detailed comparison shows that our distribution curves fall well inside the error bounds of their Monte Carlo results. This means that our result agrees with that of OST07 even quantitatively.

Figure 2 shows the evolution of the mean compact size ($a_A$) and the mean porous size ($\langle a_A \rangle_p$) for different growth models. Here, $a_\infty = (3V_\infty/4\pi t)^{1/3} = N_{bd}^{1/3} a_0$ is the compact (mass-equivalent) volume, and $(F)_m \equiv \int F(M)Mn(M)dM/\int Mn(M)dM$ is the mass-weighted average of a function $F(M)$. The mass-weighted average approximately corresponds to the value at the peak of the mass spectrum $Ma(a_\infty)n(a_\infty)$. The vertical axis $(a_A)_m/(a_\infty)_m$ is roughly equal to the third root of the mean enlargement factor, $(\psi_{enl}^{1/3})$. Comparing this figure with Figure 12 in OST07, we find excellent agreement between our evolution curves and those of OST07 except that a slight difference is seen in the late-time behavior for the porous, $\alpha_T = 10^{-2}$, model. The cross symbols in Figure 2 indicate the mean values of $a_A$ (horizontal axis) and $a_A/a_\infty$ (vertical axis) of the rain-out aggregates for the four growth models. We compare our values with those of OST07 in Table 1. Here “Smol+VA” refers to the results of our extended Smoluchowski method with the volume-averaging approximation, and “MC” refers to the results of the full 2D Monte Carlo method taken from Table 2 of OST07. We find that these values agree within errors of 10%.

From the above comparison, we conclude that our extended Smoluchowski method well reproduces the results of the Monte Carlo simulations by OST07.
3.4. Merits and Drawbacks of the Extended Smoluchowski Method

In closing this section, we point out some advantages and disadvantages of our extended Smoluchowski method over the previous Monte Carlo methods.

The most remarkable advantage of the extended Smoluchowski method is the efficiency in numerical calculations. The CPU time required for our method to perform each of the above simulations is approximately one minute on a 3GHz CPU. In contrast, Zsom & Dullemond (2008) reported that their Monte Carlo method required 10 minutes for the same simulation (the calculation of OST07 is less efficient than this since they did not use a grouping algorithm as done by Zsom & Dullemond (2008) and Ormel & Spaans (2008)). This means that our method is at least an order of magnitude more efficient than the Monte Carlo methods. The high efficiency of our method is attributed to the volume-averaging approximation we introduced in Section 2.2.

Another advantage is that we can use any numerical scheme having developed for the conventional Smoluchowski equation. For example, one can further accelerate our method just using an implicit time integration developed by Brauer et al. (2008). The implicit integration is particularly useful when one tries to include the fragmentation of aggregates that can make the problem extremely stiff in time (Brauer et al. 2008; Birnstiel et al. 2009). By contrast, the implicit integration is inapplicable to Monte Carlo methods.

There are two main drawbacks in our method. First, our method cannot be used to a problem in which the volume-averaging approximation is invalid. For example, the volume-averaging approximation will break down if a coagulation problem to be solved involves the fragmentation of aggregates and if the fragments obey broad and flat porosity distribution for each fragment mass. For this reason, we recommend improved Monte Carlo methods by Ormel & Spaans (2008) and Zsom & Dullemond (2008). Second, our Smoluchowski method is inapplicable to studying “runaway” growth in which the discreteness of the number density becomes important (Wetherill 1990). Runaway growth will be well studied by the Monte Carlo code of Ormel & Spaans (2008), which can, in principle, deal with a single aggregate.

4. A NEW HIT-AND-STICK COLLISION MODEL

The collision model of OST07 is only based on the knowledge of the porosity evolution in the BCCA and BPCA limits. This means that there are no empirical supports that validate their model for general types of aggregation. In this section, we present a new collision model based on $N$-body simulations for more general types of aggregation.

As a first step toward a comprehensive model, the present study focuses on “hit-and-stick” collisions, i.e., collisions involving neither compression nor fragmentation. The hit-and-stick approximation is valid when the collision energy $E$ is smaller than the rolling-friction energy $E_{roll}$ (Dominik & Tielens 1997; see also Section 3.1). Assuming head-on collisions between equal-sized icy aggregates (made of 0.1 $\mu$m monomers) at 5AU in a laminar MMSN, for instance, the compression and fragmentation is safely neglected until the monomer number of the aggregates becomes $\sim 10^{11}$, or the porous size becomes $\sim$cm (Suyama et al. 2008). Modeling of porosity changes as the compression and fragmentation requires $N$-body simulations that take into account the surface interaction between constituent particles, as recently done by several authors (Wada et al. 2007, 2008, 2009; Suyama et al. 2008; Paszun & Dominik 2009). At the present, this kind of simulations have been only performed for limited types of collisions (e.g., equal-sized, head-on, or low-mass collisions), and we thus have no sufficient empirical data on how the compression and fragmentation affects the porosity of resultant aggregates for more general cases. For this reason, we defer the construction of the porosity change formula beyond the hit-and-stick regime to the future work. We also neglect the rotation of aggregates during their collision for simplicity. The rotation could make the collisional outcome less compact (Krause & Blum 2004; Paszun & Dominik 2006).

The main goal of this section is to provide a reliable recipe for determining the porosity change of aggregates upon general hit-and-stick collisions. As in the previous sections, the porosity change due to a single collision is represented by the volume of the resultant aggregate, $V_{1+2}$. Without loss of generality, we may rewrite this in the form

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

(27)

where $V_1$ and $V_2(<V_1)$ are the volumes of the collided aggregates, and $\chi$ is a dimensionless factor depending on the properties of the aggregates. Since $\chi$ vanishes for the ideal compact aggregation, we can think of $\chi V_2$ as the volume of the “voids” newly created in the resultant aggregate. For this reason, we may regard $\chi$ as the void factor. As we see later, the void factor $\chi$ is constant in the BCCA and BPCA limits, suggesting that $\chi$ rather than $V_{1+2}$ is a “good” variable that describes the porosity change due to a general hit-and-stick collision. Our task is thus to present an empirical formula for the void factor $\chi$ in the hit-and-stick regime.

It is essential to prepare reliable empirical data on which the porosity change formula is to be built. For this purpose, we have performed numerical experiments on various types of collisional aggregation. Although classical BCCA and BPCA are useful aggregation models, these are just the two limiting cases of general hit-and-stick collisions. In order to bridge the gap between the two opposite limits, we introduce a new aggregation model: quasi-BCCA (QBCCA). We define QBCCA as a sequence of ballistic collisions between two clusters with a fixed mass ratio $\epsilon \equiv M_2/M_1(<1)$. Figure 3 schematically illustrates the QBCCA model as well as classical BCCA and BPCA. In the following subsections, we describe these aggregation models in more detail.

Here, we outline how we construct the collision model in this section. In Section 4.1, we introduce how the “volume” of a porous aggregate is defined in our model. In Section 4.2, we show the results of our $N$-body simulations to see how the volume of an aggregate evolves in BCCA, BPCA, and QBCCA. In Section 4.3, we synthesize these $N$-body results to obtain a single empirical formula that approximately determines the value of $\chi$ for a general hit-and-stick collision. Finally, in

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Table 1

| Model | $a_1$ (cm) | $a_1/a_\sigma$ |
|-------|------------|----------------|
| Smol+VA | MC | Smol+VA | MC |
| $a_T = 10^{-4}$, porous | 1.9 | 1.2 $\pm$ 0.1 | 4.4 | 4.4 |
| $a_T = 10^{-5}$, compact | 0.022 | 0.024 | 1 | 1 |
| $a_T = 10^{-5}$, porous | 7.6 | 7.8 $\pm$ 0.7 | 1.5 | 1.6 $\pm$ 0.1 |
| $a_T = 10^{-6}$, porous | 0.019 | 0.021 | 4.4 | 4.4 |
Section 4.4, we describe how the aerodynamical and collisional cross sections of a porous aggregate are determined in our model.

4.1. The Characteristic Radius and Volume

Since a porous aggregate is generally irregular, the concept of its “volume,” or “radius,” is somewhat ambiguous. A useful definition for the radius is the gyration radius

\[ a_g \equiv \sqrt{\frac{1}{N} \sum_{k=1}^{N} (x_k - X)^2}, \]  

(28)

where \( x_k \) \((k = 1, 2, \ldots, N)\) are the coordinates of constituent monomer and \( X = \frac{1}{N} \sum x_k \) is the coordinate of the center of mass. Another definition is the characteristic radius (Mukai et al. 1992)

\[ a_c \equiv \sqrt{\frac{5}{3} a_g} = \sqrt{\frac{5}{3N} \sum_{k=1}^{N} (x_k - X)^2}. \]  

(29)

Using \( a_c \), we can define the characteristic volume

\[ V_c = \frac{4\pi}{3} a_c^3. \]  

(30)

The characteristic radius has a property that it reduces to the physical radius for a homogeneous sphere (Mukai et al. 1992). In our model, we regard \( a_c \) and \( V_c \) as the “radius” and “volume” of a porous aggregate.\(^4\) Note that the collision model of OST07 uses the area-equivalent volume \( V_A \) (Equation (21)) and its associated radius \( a_A \) (Equation (26)).

Figure 4 shows three samples of \( N \)-body clusters created in our numerical experiments together with their “radii” measured in different ways.\(^5\) Each of the samples is composed of \( \approx 10^3 \) monomers, and hence has the compact (mass-equivalent) radius of \( a_e = N^{1/3} a_0 \approx 10a_0 \). The large circles in this figure represent the characteristic volume \( V_c \) of these samples. We see that \( a_e \), well approximates the maximum distance from the center of mass to constituent monomers, but \( a_A \) does not. This fact motivates us to define the collisional cross section using \( a_c \) rather than \( a_A \) (see Section 4.4.2).

4.2. Porosity Evolution in Various Types of Aggregation

Here, we summarize our \( N \)-body experiments on three different types of aggregation (BCCA, BPCA, and QBCCA) and derive the volume factor \( \chi \) for each of the aggregation models.

4.2.1. BCCA

BCCA is defined as a sequence of successive collisions between identical clusters (see Figure 3(a)). In the \( N \)-body experiments, we have simulated \( 10^5 \) growth sequences of BCCA. At each collisional step, we have randomly determined the impact parameter as well as the relative orientation of colliding aggregates, and followed the ballistic trajectory until

\(^4\) For monomers \((N = 1)\), we simply set \( a_e = a_0 \) and \( V_e = V_0 \).

\(^5\) In this paper, the projected area \( A \) of a cluster is calculated as the average over 15 randomly chosen orientations.
shows 10 examples of the evolution of \( a_{c,N} \) as a function of \( N \). In this figure, we also show the average of \( a_c \) over 10^5 runs. For \( N \gtrsim 30 \), the averaged \( a_c \) is found to obey a single power law

\[
a_c \propto N^{1/D_{\text{BCCA}}}, \tag{31}
\]

where \( D_{\text{BCCA}} \) is the fractal dimension of BCCA. Our data fitting shows \( D_{\text{BCCA}} \approx 1.90 \), which is consistent with the finding of previous studies (e.g., Mukai et al. 1992).

With the power-law relation (31), it is easy to find the void factor \( \chi \) for BCCA. Using Equations (30) and (31), \( V_{c,N} \) is written as

\[
V_{c,N} = \left( \frac{N_{1+2}}{N_2} \right)^{3/D_{\text{BCCA}}} V_{c,2} \approx 2.99 V_{c,2}. \tag{32}
\]

where

\[
N_{1+2} = N_1 + N_2 = 2N_2.
\]

On the other hand, Equation (27) implies \( V_{c,N} \) for BCCA. Therefore, we obtain

\[
\chi \approx 0.99 \equiv \chi_{\text{BCCA}} \tag{33}
\]

in the power-law limit. Note that \( \chi_{\text{BCCA}} \) is independent of \( V_{c,1} \).

4.2.2. BPCA

BPCA is a sequence of successive collisions between a cluster and a monomer (see Figure 3(b)). In the \( N \)-body experiments, we have simulated 10^3 growth sequences of BPCA and obtained the averaged relation between \( a_c \) and \( N \), which is plotted in Figure 5(b). For \( N \gtrsim 30 \), the \( a_c-N \) relation obeys a power law with a fractal dimension \( \approx 3.0 \), and the porosity \( P \equiv 1-V_c/V_c \) approaches to \( P_{\text{BPCA}} \approx 0.874 \). This result is consistent with the finding of previous work (Kozasa et al. 1993).

Using this result, the relation between \( V_c \) and \( N \) is written as

\[
V_c = \frac{V_c}{1-P_{\text{BPCA}}} = \frac{V_0}{1-P_{\text{BPCA}}}N. \tag{34}
\]

Since \( N_{1+2} = N_1 + 1 \), this equation implies

\[
V_{c,1+2} = V_{c,1} + \frac{V_0}{1-P_{\text{BPCA}}}. \tag{35}
\]

On the other hand, Equation (27) implies \( V_{c,1+2} = V_{c,1} + (1 + \chi) V_0 \) for BPCA. Therefore, we obtain

\[
\chi = \frac{1}{1-P_{\text{BPCA}}} - 1 \approx 6.94 \equiv \chi_{\text{BPCA}}, \tag{36}
\]

for the power-law limit. \( \chi_{\text{BPCA}} \) is independent of \( V_{c,1} \) and \( V_{c,2} \). Equation (36) is valid as long as \( N \gtrsim 30 \), or \( V_{c,1} \gtrsim (30/1-P_{\text{BPCA}}) V_0 \approx 240 V_0 \).

4.2.3. QBCCA

QBCCA is defined as a sequence of successive collisions between two clusters with a fixed mass ratio \( \epsilon < 1 \). It is clear that BCCA corresponds to QBCCA of \( \epsilon = 1 \). It is also true that BPCA asymptotically approaches to QBCCA of \( \epsilon \to 0 \) in the limit of \( N_1 \to \infty \). Therefore, this type of aggregation can be considered as a model between the BCCA and BPCA limits.

We here describe the general procedure of QBCCA. Let us refer to the larger cluster as the “target,” and to the smaller one as the “projectile.” A projectile is chosen from the outcomes of previous collisions so that the mass ratio between the target and the projectile is always a monomer. In order to obtain a “truly” QBCCA cluster, one needs to repeat the above procedure until the cluster grows beyond \( N \approx 1/\epsilon \).

Figure 3 illustrates an example of QBCCA in the case of \( \epsilon = 0.6 \). The first step is the collision between two monomers, as is for any \( \epsilon \). The second collision is between the resultant dimer \( (N_1=2) \) and a monomer \( (N_2=1) \), since \( N_2 = 1 \) is nearer to \( N_1 \epsilon = 1.2 \) than \( N_2 = 2 \). The third collision is between the resultant trimer \( (N_1=3) \) and a dimer \( (N_2=2) \), since \( N_2 = 2 \) is the nearest to \( N_1 \epsilon = 1.8 \) among \( N_2 = 1, 2, \) and 3.

In the \( N \)-body experiments, we have chosen eight values of \( \epsilon \) from the range 0.005 < \( \epsilon < 1.0 \). For each value of \( \epsilon \), we have simulated 100–2000 growth sequences and obtained an averaged \( a_c-N \) relation. Figure 5(b) shows two examples of the averaged relations (\( \epsilon = 0.05 \) and 0.005). The averaged relations roughly obey a power law

\[
a_c \propto N^{1/D_{\text{QBCCA}}(\epsilon)}, \tag{37}
\]
for $N > 1/\epsilon$, where $D_{\text{QBCCA}}(\epsilon)$ is the fractal dimension of the QBCCA clusters and depends on the mass ratio $\epsilon$. For each value of $\epsilon$, we measured $D_{\text{QBCCA}}$ by fitting the power law (37) to the corresponding curve in Figure 5(b). Detailed inspection shows that the averaged curves for QBCCA logarithmically oscillate around the power-law fits with a cycle $\Delta \log N \sim \log(1/\epsilon)$. This is an imprint of the history that clusters of $N \lesssim 1/\epsilon$ are not constructed by the "truly" QBCCA process. We neglect this oscillation in the following modeling since the amplitude is small.

The obtained values of $D_{\text{QBCCA}}$ as well as $D_{\text{QBCCA}}(1) \equiv D_{\text{BCCA}}$ are plotted in Figure 6. Remarkably, $D_{\text{QBCCA}}(\epsilon)$ differs from $D_{\text{BCCA}}$ by only 10% even for $\epsilon \sim 10^{-2}$, or $V_{c,2}/V_{c,1} \sim (10^{-2})^{3/D_{\text{QBCCA}}} \sim 10^{-3}$. This suggests that an aggregate growing by hit-and-stick collisions tends to have a fractal dimension close to 2 unless its collision partners are much smaller than itself. A simple linear extrapolation of the curve in Figure 6 suggests that $D_{\text{QBCCA}}(\epsilon)$ will approach to 3 if $\epsilon$ (or $V_{c,2}/V_{c,1}$) is set to be as small as $10^{-7}$.

Equation (37) implies a relation similar to Equation (32),

$$V_{c,1+2} = \left( \frac{N_{1+2}}{N_1} \right)^{3/D_{\text{QBCCA}}(\epsilon)} = (1 + \epsilon)^{3/D_{\text{QBCCA}}(\epsilon)}, \quad (38)$$

where we have used $N_{1+2} = (1 + \epsilon)N_1$. We can express this equation as a function of $V_{c,2}/V_{c,1}$ instead of $\epsilon$. First, we note that Equation (37) also implies

$$\epsilon = \left( \frac{V_{c,2}}{V_{c,1}} \right)^{D_{\text{QBCCA}}(\epsilon)/3}. \quad (39)$$

Since $D_{\text{QBCCA}}$ is a function of $\epsilon$, Equation (39) determines $\epsilon$, and consequently $D_{\text{QBCCA}}$, as a function of $V_{c,2}/V_{c,1}$. Using Equation (39), Equation (38) is written as

$$V_{c,1+2} = \left[ 1 + \left( \frac{V_{c,2}}{V_{c,1}} \right)^{D_{\text{QBCCA}}(\epsilon)/3} \right]^{3/D_{\text{QBCCA}}} V_{c,1}. \quad (40)$$

Thus, the void factor $\chi$ for QBCCA is given by

$$\chi = \left[ 1 + \left( \frac{V_{c,2}}{V_{c,1}} \right)^{D_{\text{QBCCA}}(\epsilon)/3} \right]^{3/D_{\text{QBCCA}}} - 1 \approx \chi_{\text{QBCCA}}(V_{c,2}/V_{c,1}). \quad (41)$$

Since $D_{\text{QBCCA}}$ is a function of $V_{c,2}/V_{c,1}$, $\chi_{\text{QBCCA}}$ only depends on $V_{c,2}/V_{c,1}$.

Figure 7 shows the void factor $\chi_{\text{QBCCA}}$ as a function of $2V_{c,2}/(V_{c,1} + V_{c,2}) = 2/(V_{c,1}/V_{c,2} + 1)$. We see that $\chi_{\text{QBCCA}}$ scales linearly with $2V_{c,2}/(V_{c,1} + V_{c,2})$. By data fitting, we obtain a simple empirical formula

$$\chi_{\text{QBCCA}}(V_{c,2}/V_{c,1}) \approx \chi_{\text{BCCA}} - 1.03 \ln \left( \frac{2}{V_{c,1}/V_{c,2} + 1} \right). \quad (42)$$

where $\chi_{\text{BCCA}}$ is given by Equation (33). Note that this formula includes the BCCA limit since it gives $\chi_{\text{QBCCA}} = \chi_{\text{BCCA}}$ for $V_{c,1} = V_{c,2}$. Also note that, although $\chi_{\text{QBCCA}}$ increases as $V_{c,2}$ decreases, the void volume $\chi_{\text{QBCCA}} V_2$ decreases with decreasing $V_{c,2}$.
4.3. A Recipe for Porosity Change Due to General Hit-and-stick Collisions

Figure 7(b) summarizes $X_{\text{BCCA}}$, $X_{\text{BPCA}}$, and $X_{\text{QBCCA}}$ as a function of $2V_2/(V_1 + V_2) = 2/(V_1/V_2 + 1)$. Note that $X_{\text{BPCA}}$ is only plotted in the range $V_{c,2}/V_{c,1} < 1/240$, since the $a_c/N$ relation for BPCA obeys a power law only when $V_{c,2}/V_{c,1} \gtrsim 1/240$ (see Section 4.2.2).

Now we combine the above results to construct a recipe of the void factor $\chi$ for general hit-and-stick collisions. In the previous subsection, we have seen that $\chi$ can be simply written as a function of only $V_{c,2}/V_{c,1}$ under a fixed aggregation process (i.e., BCCA/QBCCA/BPCA). This can be done because $N_2/N_1$ is related to $V_{c,2}/V_{c,1}$ for each process. This simplicity is appealing for the modeling of the porosity change. For this reason, we assume that the growth history of an aggregate is well approximated either by successive collisions of a fixed volume ratio $V_{c,2}/V_{c,1}$ (BCCA/QBCCA) or by successive collisions of a fixed projectile volume $V_2$ (BPCA). This assumption allows us to choose $\chi$ between $X_{\text{QBCCA}}(V_{c,2}/V_{c,1})$ and $X_{\text{BPCA}}$. We will discuss the validity of this assumption in Section 5.3. Next, we determine the choice so that the value of $\chi$ reduces to $X_{\text{BCCA}}$ and $X_{\text{BPCA}}$ in the limit of $V_{c,2}/V_{c,1} \to 1$ and 0, respectively. Among the simplest ones, we propose the following formula:

$$\chi(V_{c,2}/V_{c,1}) = \min(X_{\text{QBCCA}}(V_{c,2}/V_{c,1}), X_{\text{BPCA}}),$$

(43)

where $X_{\text{BPCA}}$ and $X_{\text{QBCCA}}(V_{c,2}/V_{c,1})$ are given by Equations (36) and (42), respectively. This final formula is illustrated in Figure 7(b) by the thick gray line. It should be noted here that the above choice underestimates the porosity increase for QBCCA with very small $V_{c,2}/V_{c,1}$. However, as seen in Section 5.2, this effect is negligibly small.

It is worth trying to compare our hit-and-stick model with that of the OST07. Unfortunately, we cannot make a rigorous comparison between the two models here since the OST07 model considers the porosity increase using $V_A$. However, it is possible to derive the “area-equivalent void factor” $\chi_A$ for the OST07 model by equating their hit-and-stick formula (23) and $V_{A,1+2} = V_{A,1} + (1 + \chi_A) V_{A,2}$. Neglecting $\psi_{\text{add}}$ in Equation (23) (which is negligible as long as $N_1, N_2 \gg 10^3$), we obtain

$$\chi_{A,\text{OST07}}(V_{A,2}/V_{A,1}) = \frac{V_{A,1}}{V_{A,2}} \left[ \frac{V_{A,2}}{V_{A,1}} \right]^{2\chi_{\text{CCA}}/3} - 1 \right]^{-1} - 1,$$

(44)

Note that $\chi_{A,\text{OST07}}$ depends on $V_{A,2}/V_{A,1}$ only. In Figure 7(b), we overplot $\chi_{A,\text{OST07}}$ as a function of $2V_{A,2}/(V_{A,1} + V_{A,2})$. We see that $\chi_{A,\text{OST07}}$ is approximately equal to $\chi$ of our model in the BCCA limit, but decreases for smaller $V_{A,2}/V_{A,1}$. As shown in Section 5, the OST07 model considerably underestimates the porosity increase of aggregates because of this behavior.

Summarizing Sections 4.2 and 4.3, we have constructed the porosity change recipe for general hit-and-stick collisions in accordance with numerical experiments on various types of aggregation. In the numerical experiments, a new aggregation model, which we have referred as QBCCA, has been used to fill the gap between the conventional BCCA and BPCA models. The porosity change recipe has been given in the form of a formula for the “void factor” $\chi$ (Equation (43)), which eventually determines the volume of a collisionally formed aggregate, $V_{i+2}$, via Equation (27). This recipe thus allows us to evaluate the porosity change of aggregates upon a single hit-and-stick collision. One can calculate the growth and porosity evolution of an ensemble of dust aggregates consistently by implementing this recipe to the Monte Carlo methods or the extended Smoluchowski method presented in Section 2.

4.4. Cross Section Formulae

The porosity of aggregates affects the aerodynamical (projected) cross section $A$ and the collisional cross section $\sigma_{\text{coll}}$. Below, we describe how we calculate these cross sections in our collision model.

4.4.1. Projected (Aerodynamical) Cross Section

The projected cross section $A$ is one of the most important properties of an aggregate since it determines how strongly the aggregate is coupled to gas environment.

It is useful to see how the projected cross section behaves differently in BCCA and BPCA. In the BCCA limit, $A$ is well approximated by Minato et al. (2006)

$$\frac{A_{\text{BCCA}}}{A_0} \approx \left\{ \begin{array}{ll}
12.5 N^{0.685} \exp(-2.53/N^{0.0920}), & N < 16,
\end{array} \right.$$

$$0.352 N + 0.566 N^{0.862}, \quad N \geq 16,$$

(45)

where $A_0 = \pi a_0^2$ is the geometrical cross section of a monomer. To see how accurately this formula predicts the actual value of $A$, we take the BCCA cluster in Figure 4 as an example. This cluster contains $N = 1024$ monomers, and the angle average of its projected area is $A = 1890a_0^2$ (the area-equivalent radius being $a_A = 24.5 a_0$). The empirical formula, Equation (45), gives $A_{\text{BCCA}} = 1830 a_0^2$ ($a_A = 24.1 a_0$), which agrees with the above actual value with a relative error of 3.3%. We remark here that the area-equivalent radius $a_A$ of a BCCA cluster is generally much smaller than its characteristic radius $a_c$. For example, the BCCA cluster shown in Figure 4 has $a_c = 61.1 a_0$, which is about three times larger than its $a_A$. In fact, the “characteristic” cross section of a BCCA cluster, $\pi a_c^2 \approx N^{2}/P_{\text{BCCA}} A_0 \approx N^{1.05} A_0$, increases faster than the total geometric cross section of constituent monomers, $N a_0$. This means that if we naively assumed $A = \pi a_c^2$ in our collision model, we would have a BCCA cluster more and more strongly coupled to gas as its growth. In contrast, the formula, Equation (45), guarantees that $A$ does not increase faster than $N a_0$.

In the BPCA limit, $A$ is simply related to $a_c$ as

$$A_{\text{BPCA}} \approx \pi a_c^2,$$

(46)

or equivalently, $a_A \approx a_c$. For example, the BPCA cluster shown in Figure 4 has the angle-averaged projected cross section of $A = 1080 a_0^2$, or the area-equivalent radius of $a_A = 18.5 a_0$. The characteristic radius of this cluster is $a_c = 19.2 a_0$, and thus the relative difference between $a_A$ and $a_c$ is only 4%.

Using the above facts, we construct a formula for $A$ of a general porous aggregate. Let us take the general formula to approximately recover Equations (45) and (46) in the BCCA and BPCA limits. As one of the simplest ones, we consider

$$A(N, a_c) = \left( \frac{1}{A_{\text{BCCA}}(N)} + \frac{1}{\pi a_c^2} - \frac{1}{\pi a_{c,\text{BCCA}}^2(N)} \right)^{-1},$$

(47)

where $A_{\text{BCCA}}(N)$ is the fitting formula defined by Equation (45) and $a_c, A_{\text{BCCA}}(N)$ is the averaged characteristic radius of BCCA clusters of the same monomer number $N$. This formula clearly reduces to Equation (45) in the BCCA limit, and also recovers Equations (46) in the BPCA limit for large $N$ where $a_c^2 \ll A_{\text{BCCA}}$. 
and \(a_c \ll a_{c,BCCA}\). The upper panel of Figure 8 shows the accuracy of this formula for more general types of clusters. In this figure, the solid curves represent the averaged relation between the mass \(N\) and the mass-to-area ratios \(N/A\) obtained for various BCCA/QBCCA models (\(\epsilon = 1, 0.325, 0.1, 0.05, \) and 0.01). The dashed curves are obtained from Equation (47) with the averaged \(a_c - N\) relations for our BCCA/QBCCA clusters. For \(N \lesssim 10^6\), the relative error between the measured values and the prediction from Equation (47) is less than 20\% for \(\epsilon \geq 0.05\) and less than 30\% even for \(\epsilon = 0.01\). Thus, Equation (47) successfully converts \(a_c\) into \(N\).

Recently, Paszun & Dominik (2009) have proposed another simple relation between \(a_A\) and the outer radius \(a_{out}(\approx a_c)\), which reads (see Equation (5) in Paszun & Dominik 2009)

\[
N \left( \frac{a_0}{a_A} \right)^3 = 1.21 \left( \frac{a_{out}}{a_A} \right)^{-0.3} N^{-0.33},
\]

(48)
or \(A \propto (N^{1.33} a_{out}^{-0.3} \epsilon)^{3/3}.\) They obtained this formula from relatively small (\(N \lesssim 10^3\)) numerical aggregates.

The lower panel of Figure 8 examines the accuracy of this formula for larger \(N\). The solid curves are the same as those in the upper panel of Figure 8, but the dashed curves are now the prediction from Equation (48) with \(a_{out}\) approximated by \(a_c\). We see that the formula of Paszun & Dominik (2009) underestimates the projected area of large (\(N \gtrsim 10^3\)) BCCA/QBCCA clusters, especially for \(\epsilon \gtrsim 0.05\).

### 4.4.2. Collisional Cross Section

We explained in Section 4.1 that the characteristic radius \(a_c\) of a porous aggregate well approximates the maximum distance from the center of mass to the constituent monomers. It will be reasonable to regard two aggregates as collided if the impact parameter is smaller than the sum of their characteristic radii. For this reason, we model the collisional cross section \(\sigma_{coll}\) for two porous aggregates as

\[
\sigma_{coll} = \pi (a_{c,1} + a_{c,2})^2,
\]

(49)
where \(a_{c,1}\) and \(a_{c,2}\) are the characteristic radii of the aggregates. Note that this choice differs from that of OST07, \(\sigma_{coll} = \pi (a_{A,1} + a_{A,2})^2\).

We remark here that Equation (49) ignores the possibility that a collision can be missed even if the impact parameter is less than \(a_{c,1} + a_{c,2}\). Such collision misses frequently occur when colliding aggregates are so fluffy that their fractal dimensions are much lower than two. For example, a microgravity experiment of Krause & Blum (2004) implies that the choice of OST07 agrees the actual collisional cross section better than ours when the fractal dimension \(D\) of aggregates is as low as 1.4. However, the neglect of collision misses does not cause a serious overestimation of \(\sigma_{coll}\) in our model since we only deal with aggregates of \(D > 1.9\).

### 5. COMPARISON OF THE HIT-AND-STICK COLLISION MODELS

In Section 5, we have constructed a new collision model for porous dust aggregates. To compare this model with the classical compact model and the model by OST07, we apply the three models to solve simple problems on porous dust coagulation.

We consider two types of coagulation problems. In the first type, the coagulation is purely driven by Brownian motion. In the second type, the coagulation is driven by Brownian motion plus relative velocity of the form \(\Delta u = g[\tau_{f,1} - \tau_{f,2}]\), where \(g\) is a constant and \(\tau_{f,1}\) and \(\tau_{f,2}\) are the stopping times of two colliding aggregates. For example, sedimentation of aggregates under a gravitational field \(g\) leads to this type of relative velocity. Another important example is the relative motion driven by turbulence in the strong coupling limit (Weidenschilling 1984; Ormel & Cuzzi 2007), where \(g\) means the typical acceleration of the smallest turbulent eddies. In the following, we refer to relative motion leading to the above form of \(\Delta u\) as differential drift.

We solve the above coagulation problems using the extended Smoluchowski Equations (15) and (16). Table 2 summarizes

![Figure 8. Mass-to-area ratio \(N/A\) of BCCA and QBCCA clusters as a function of monomer number \(N\). Upper panel: the solid curves show the directly measured values averaged over \(10^2-10^6\) samples for various values of \(\epsilon (=1, 0.325, 0.1, 0.05, \) and 0.01) from bottom to top). The oscillation seen in the curves for small \(\epsilon\) is an imprint of the BPCA-like growth history for \(N \lesssim 1/\epsilon\) (see Section 4.2.3). The dashed curves show the values calculated from our simple formula \(A(N, a_c)\) (Equation (47)) together with the averaged \(a_c - N\) relations. The good agreement between the solid and dashed curves implies that the projected cross section is well modeled by Equation (47) as a function of \(a_c\) and \(N\). Lower panel: the solid curves are the same as those in the upper panel, but the dashed curves are obtained from Equation (5) of Paszun & Dominik (2009; Equation (48) in the present paper) with \(a_{out} = a_c\). The formula by Paszun & Dominik (2009) underestimates the real projected area for very large \(N\).](image-url)
the three hit-and-stick models to be compared in this section. Here \( V \) refers to the volume to be evolved by Equation (16). Note that the characteristic volume \( V_c \) is identical to the area-equivalent volume \( V_A \) in the classical compact model. Since the OST7 model gives no relation between \( V_c \) and \( V_A \), we use the projected area \( A \) when we compare the porosity evolution of the three models. We set \( a_{ac,BCCA}(N) = a_0 N^{1/D_{ac}} \), when we use Equation (47) in our model.

5.1. Coagulation Driven by Brownian Motion

The mean relative velocity driven by Brownian motion is written as

\[
\Delta u_B = u_{B0} \sqrt{\frac{1}{N_1} + \frac{1}{N_2}},
\]

where \( u_{B0} = \sqrt{8 k_B T / \pi m_0} \) is the thermal velocity of a monomer. \( \Delta u_B \) is independent of the projected area \( A \) of colliding aggregates, so the area formula in our model does not affect the coagulation. Kempf et al. (1999) performed a full \( N \)-body simulation of Brownian-motion-driven coagulation and found that the resultant aggregates have fractal dimensions \( D \approx 1.8 \pm 0.2 \). We use this fact to examine the validity of our collision model.

In the numerical simulations, we start with a monodisperse ensemble of monomers and followed the evolution of \( n(M) \) and \( \nabla \langle M \rangle \) using Equations (6) and (7). The control parameters are set to \( N_{tot} = 80 \) and \( \delta = 0.05 \).

Figure 9 shows the normalized mass distribution functions \( N^2 n(N)/n_0 \) at time \( t = 10^4 t_{B0} \) obtained from the three collision models. Here, \( n_0 \) and \( t_{B0} = t_{B0} \) are the number density and growth rate of monomers at the initial moment among the models. Note that the mass conservation ensures \( \int (N^2 n(N)/n_0) d\ln N = 1 \). We find that the shape of the distribution function is insensitive to the choice of the models. However, the growth rates of the aggregates are quite different among the models. At this time, the mass-weighted average mass \( \langle M \rangle_m \) is \( 10^{5.7} m_0 \), \( 10^{6.9} m_0 \), and \( 10^{5.5} m_0 \) for the compact, OST7, and our models, respectively (see Section 3.3 for the definition of \( \langle M \rangle_m \)). This is essentially due to the difference in the porosity evolution among the three models (see Figure 11 below); namely, the higher porosity results in the larger collisional cross section, and thus the faster growth rate.

Figure 10 shows the snapshots of the mean internal density \( \rho_c(M) = M/V_c(M) \) at \( t = 10^4 t_{B0} \) for the compact model and our model. We find that the density curve for our model is well represented by a single power law \( \rho_c \propto M^{1-D/D_{ac}} \) with \( D = 1.96 \). This means that the aggregates resulting from our model have a fractal dimension of 1.96, which is consistent with

\[
\begin{array}{|c|c|c|c|}
\hline
\text{Model} & V & V_{1+2} & A \\hline
\text{Compact} & V_c & V_{c1} + V_{c2} & A_0 N^{1+D/3} \\hline
\text{OST7} & V_A & \text{Equation (23)} & A_0 (V_A / V_B)^{1+D/3} \\hline
\text{Our model} & V_c & \text{Equations (27) and (43)} & A_0 (a_{ac}^2)^{1+D/3} \\hline
\end{array}
\]
the finding of Kempf et al. (1999). Thus, our model successfully reproduces the porosity evolution of aggregates growing in Brownian motion. We also plot the density curve for our model at earlier moment, \( t = 10^2 t_0 \). The curve again lies on the same fractal line, meaning that the fractal dimension of the aggregates does not change with time.

The difference between the OST07 model and ours is best illustrated by the evolution of projected area \( A \). Figure 11 shows the normalized mass-to-area ratio \( N/(A/A_0) \) for the three collision models at \( t = 10^4 t_0 \) as a function of \( N \). We see that the OST07 model gives a considerably small projected area for growing aggregates compared with our model. At this moment, the aggregates of the OST07 model with mass \( (M)_m \) have a projected area approximately an order of magnitude smaller than our aggregates of the same mass. The underestimation of \( A \) in the OST07 model is clearly caused by the decreasing behavior of \( x_{A,\text{OST07}} \) for \( V_{A,2}/V_{A,1} < 1 \). Thus, the realistic modeling of the porosity change between the BCCA and BPCA limits is critical.

5.2. Coagulation Driven by Differential Drift

We consider aggregates smaller than the mean free path of the ambient gas, and adopt the Epstein’s law \( \tau_f \propto M/A \). Then, the relative velocity induced by differential drift is written as

\[
\Delta u_\Delta = u_{D0} \left| \frac{N_1}{A_1/A_0} - \frac{N_2}{A_2/A_0} \right|, \tag{51}
\]

where \( u_{D0} = g \tau_0 \) is the drift velocity of monomers. Wurm & Blum (1998) conducted a laboratory experiments on dust coagulation in a turbulent gas environment and showed that the resultant aggregates have a fractal dimension of \( D \approx 1.91 \).

As in Section 5.1, we start the simulations with a monodisperse ensemble of monomers. However, pure differential drift cannot drive the first step of the coagulation because \( \Delta u_\Delta \) vanishes for all pairs of monomers. To avoid this, we add \( \Delta u_B \) as a small perturbation and take the relative velocity to be

\[
\Delta u = \sqrt{\Delta u^2_\Delta + \Delta u^2_B} \text{ with } u_{B0} = 0.1 u_{D0}.
\]

The inclusion of \( \Delta u_B \) does not affect the dust evolution at a later time since \( \Delta u_B \) decreases as the aggregates grow. The simulations are performed with the control parameters \( N_{\text{col}} = 80 \) and \( \delta = 0.01 \). Time evolution is followed until \( t = 20 t_{D0} \), where \( t_{D0} = \left( n_{D0} A_0^2 u_{D0}/\pi D_0 \right)^{-1} \).

Figure 12 compares the mass distributions \( N^2 n(N)/n_0 \) for the three collision models at \( t = 20 t_{D0} \). The average mass \( (M)_m \) at this moment is \( 10^{13.8}m_0, 10^{10.3}m_0, \) and \( 10^{8.6}m_0 \) for the compact, OST07, and our models, respectively. In contrast to the Brownian motion case, our model results in the slowest increase in \( (M)_m \) among the three models. This is because our aggregates tends to conserve the mass-to-area ratio \( N/A \), and thus keep \( \Delta u_\Delta \propto \Delta(N/A) \) small, throughout the growth.

Figure 13 shows the snapshot of the \( \rho-M \) relations at \( t = 20 t_{D0} \) for the compact model and our model. We see that the density curve for our model behaves differently between the low-mass \( (M \lesssim (M)_m) \) and high-mass \( (M \gtrsim (M)_m) \) sides. At the low-mass side, the density curve again obeys a power-law relation. The fractal dimension for this side is found to be \( D = 2.09 \), which agrees with the finding of Wurm & Blum (1998) within an error of 10%. The fractal dimension obtained here is slightly higher than that in the Brownian motion case. This is because the differential drift inhibits equal-sized collisions (see Equation (51)) and the dominant collision mode shifts to lower \( \epsilon \). Comparing the obtained fractal dimension \( D = 2.09 \) with \( D_{\text{BCCA}}(\epsilon) \) in Figure 6, the mass ratio of the dominant collisions is estimated as \( \epsilon \approx 0.05 \). We discuss, in more detail, the dominant collision mode in the differential drift as well as Brownian motion in Section 5.3.

At the high-mass side, in contrast, the density curve deviates from the above power-law relation and tends to flatten. We observe this behavior independently of \( t \), as is found from the density curve at earlier time \( t = 10t_{D0} \) plotted in Figure 13. This implies that the growth history of massive aggregates is qualitatively different from that of smaller ones when the coagulation is driven by the differential motion. In fact, this high-mass behavior can be explained if we suppose that (1) typical-mass aggregates grow by the collision with similar-sized ones, while (2) the massive aggregates grow by the collision with much smaller, typical-sized \( (M \sim (M)_m) \) ones. For simplicity, let us divide an ensemble of aggregates into two classes, one being a small number of massive aggregates with mass \( M_1 \gg (M)_m \), and the other being a large population of typical aggregates with mass \( M_2 \sim (M)_m \). We ignore the collision between massive aggregates and assume that the both classes of aggregates grow only by colliding with typical ones.
In addition, we assume that the both classes of aggregates grow at the same rate, i.e.,

\[
\frac{1}{M_1} \frac{dM_1}{dt} = \frac{1}{M_2} \frac{dM_2}{dt} = \frac{1}{t_{\text{grow}}},
\]

(52)

where \(t_{\text{grow}}^{-1}\) is the growth rate independent of \(M\). Under these assumptions, the increase in the volume \(V_2\) of a typical-mass aggregate is given by the rate of collisions with other typical-mass aggregates, \(v_{\text{coll},2} = (dM_2/dt)/M_2 = t_{\text{grow}}^{-1}\), times the volume increase per collision, \([1 + \chi(V_2/V_1)]V_2\), i.e.,

\[
\frac{dV_2}{dt} = \frac{1 + \chi_{\text{BCCA}}}{t_{\text{grow}}} V_2,
\]

(53)

where we have used that \(\chi(V_2/V_1) = \chi_{\text{BCCA}}\). Meanwhile, the increase in the volume \(V_1\) of a high-mass aggregate is given by the rate of collisions with typical-mass aggregates, \(v_{\text{coll},12} = (dM_1/dt)/M_1 = (M_1/M_2)t_{\text{grow}}\), times the volume increase per collision, \([1 + \chi(V_2/V_1)]V_1\), i.e.,

\[
\frac{dV_1}{dt} = \frac{M_1}{M_2} \frac{1 + \chi(V_2/V_1)}{t_{\text{grow}}} V_2 = \frac{\rho_1}{\rho_2} \frac{1 + \chi(V_2/V_1)}{t_{\text{grow}}} V_1,
\]

(54)

where we have used that \(\rho = M/V\). Using Equations (52)–(54), the time variation of \(\rho_1/\rho_2\) is written as

\[
\frac{d\ln(\rho_1/\rho_2)}{dt} = \frac{1}{M_1} \frac{dM_1}{dt} - \frac{1}{V_1} \frac{dV_1}{dt} - \left( \frac{1}{M_2} \frac{dM_2}{dt} - \frac{1}{V_2} \frac{dV_2}{dt} \right) = - \frac{1}{V_1} \frac{dV_1}{dt} + \frac{1}{V_2} \frac{dV_2}{dt} = \frac{1}{t_{\text{grow}}} \left[ 1 + \chi_{\text{BCCA}} - \frac{\rho_1}{\rho_2} [1 + \chi(V_2/V_1)] \right].
\]

(55)

The solution to this equation asymptotically satisfies \(d(\rho_1/\rho_2)/dt = 0\), or

\[
\rho_1 = \frac{1 + \chi_{\text{BCCA}}}{1 + \chi(V_2/V_1)} \rho_2 = \frac{1 + \chi_{\text{BCCA}}}{1 + \chi(V_2/V_1)} \frac{M_1/M_2}{\rho_1/\rho_2} \rho_2.
\]

(56)

For fixed \(M_2\) and \(\rho_2 = \rho(M_2)\), this final equation implicitly determines \(\rho_1\) as a function of \(M_1\). In Figure 13, we overplot the solutions \(\rho_1\) to Equation (56) at \(t = 10t_{\text{D0}}\) and \(20t_{\text{D0}}\) as a function of \(M_1\) with \(M_2 = \langle M \rangle_m\) and \(\rho_2 = \rho(\langle M \rangle_m)\). We find that these solutions reproduce the flattening of the density profiles. The flattening of the density curve is intuitively reasonable, since the porosity of an aggregate is generally kept small when it only accretes much smaller aggregates.

Figure 14 compares the normalized mass-to-area ratios \(N/(A/A_0)\) for the two collision models at \(t = 20t_{\text{D0}}\) as a function of \(M\). The mass-to-area ratio is a key property of aggregates growing by differential drift since the terminal velocity is proportional to it. Again, the \(M/A-M\) relation for our model exhibits different behavior between the low-mass \((M \lesssim \langle M \rangle_m)\) and high-mass \((M \gtrsim \langle M \rangle_m)\) sides: nearly flat in the low-mass side and increasing with mass in the high-mass side. This difference clearly reflects the \(\rho-M\) relation seen in Figure 13.

---

6 This assumption works well when the coagulation is driven by the differential drift. In this case, \(dM/dt = \rho_0\sigma_{\text{coll}}\Delta t_{\text{D0}}\) scales with \((\sigma_{\text{coll}}/A)M\), so \(t_{\text{grow}}^{-1}\) scales with \(\sigma_{\text{coll}}/A\). However, \(\sigma_{\text{coll}}\) is roughly proportional to \(A\), and therefore \(t_{\text{grow}}^{-1}\) is approximately constant.

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In Figure 14, Snapshot of the normalized mass-to-area ratios \(N/(A/A_0)\) at \(t = 20t_{\text{D0}}\) for the differential-drift-driven coagulation with different collision models. The open circles indicate the mass-weighted average masses \(\langle M \rangle_m\). Moreover, detailed inspection shows that \(M/A\) for the OST7 model also steepens in the high-mass end. Thus, the steepening of the \(M/A\) curve is not peculiar to our model.

One might suspect that the increase in the mass-to-area ratio is caused by the cutoff in the void factor \(\chi\) (Equation (43)) at small \(V_2/V_1\). Actually, the complete flattening as seen in Figure 13 is achieved because we have chosen \(\chi = \chi_{\text{BCCA}}\) in the small \(V_2/V_1\) limit (see Section 4.3). This can be confirmed from Equation (56), which implies \(\rho_1 \rightarrow \rho_2 (1 + \chi_{\text{BCCA}})/(1 + \chi_{\text{BPCA}}) \approx 0.25\rho_2\) independently of \(V_1\). However, flattening still occurs even if we choose \(\chi = \chi_{\text{BPCA}}(V_2/V_1)\) for all \(V_2/V_1\). In fact, Equation (56) then implies \(\rho_1 \propto 1/\log(V_1/V_2)\) in the small \(V_2/V_1\) limit, which decreases only logarithmically with increasing \(V_1\). For confirmation, we have solved the same coagulation problem by removing the cutoff in \(\chi\) and assuming \(\chi = \chi_{\text{BCCA}}(V_2/V_1)\) for all \(V_2/V_1\). The result is overplotted in Figure 14. We see that \(M/A\) at the high-end is mostly unchanged even if the cutoff in \(\chi\) is removed. Thus, the increase of the mass-to-area ratio seems to be a robust feature for the coagulation driven by the differential drift.

The above finding has a potentially important implication for the growth of dust aggregates in protoplanetary disks. One of the authors has recently examined the effect of dust charging on its collisional growth in protoplanetary disks (Okuzumi 2009). Aggregates in a disk usually charge up negatively on average, and their collisions require a sufficiently high collision velocity to overcome the electrostatic barrier. Strikingly, it turned out that the electrostatic repulsion strongly suppresses the growth of fractal \((D \approx 2)\) aggregates. This is essentially because a fractal aggregate of \(D \approx 2\) keeps a small mass-to-area ratio and thus a low sedimentation velocity. However, our calculation shows that high-mass aggregates in an ensemble have a large mass-to-area ratio and a high sedimentation velocity compared with low-mass fractal aggregates. This implies that the high-mass aggregates may be allowed to continue growing even if the others are not allowed. In a forthcoming paper, we will...
investigate this issue using the numerical tools presented in this study.

5.3. Validity and Possible Limitation of Our Porosity Evolution Formula

In the modeling of the porosity evolution, we have assumed that the growth of an aggregates is well approximated as BCCA/QBCCA or BPCA. Here, we examine whether this assumption holds in the above coagulation problems.

Let us consider a quantity

\[ C_{N_1}(\epsilon) \equiv \frac{\epsilon K(\epsilon N_1; N_1)n(\epsilon N_1)}{\int_0^{N_1} \epsilon K(\epsilon' N_1; N_1)n(\epsilon' N_1)d\epsilon'}, \quad (57) \]

where \( K(\epsilon N_1; N_1)n(\epsilon N_1) \) is the rate of collisions between aggregates with mass \( \epsilon N_1 \) and \( N_1 \). The growth rate \( t^{-1}_{\text{grow}} = (dN_1/dt)/N_1 \) of an aggregate with mass \( N_1 \) is written as \( t^{-1}_{\text{grow}} = \int_0^{N_1} \epsilon K(\epsilon' N_1; N_1)n(\epsilon' N_1)d(\epsilon' N_1). \) Thus, \( C_{N_1}(\epsilon) \) measures how collisions of mass ratios between \( \epsilon \) and \( \epsilon + d\epsilon \) contribute to the growth of an aggregate of mass \( N_1(\geq N_1) \). Figure 15 plots \( C_{(N_1)}(\epsilon) \) for Brownian motion and differential drift at different times \( t \). For both the cases, the functional form of \( C_{(N_1)}(\epsilon) \) is nearly independent of \( t \) and has a peak at \( \epsilon = 1 \) (Brownian motion case) and \( \epsilon \sim 0.1 \) (differential drift case). The distribution of \( C_{(N_1)}(\epsilon) \) has an order-of-magnitude spread in \( \epsilon \)-space. However, this spread can be regarded as narrow since an order-of-magnitude fluctuation in \( \epsilon \) only causes \( \sim 10\% \) fluctuation in \( D_{\text{QBCCA}} \) (see Figure 6). Therefore, the growth of aggregates is indeed well approximated as BCCA/QBCCA when the coagulation is driven by Brownian motion and differential drift.

On the other hand, the assumption may become less good if the collision partners of an aggregate have widely spread mass ratios if they contribute equally to its growth. Such a situation may be realized when, for example, the collision partners obey a very broad and flat size distribution.

6. SUMMARY

In this study, we have presented new numerical tools for studying the coagulation and porosity evolution of dust aggregates. Our findings are summarized as follows.

1. We have presented a new numerical method for simulating the coagulation and porosity evolution of dust aggregates as an extension of the conventional Smoluchowski method (Section 2). The new method treats the averaged volume of aggregates of the same mass as dynamical, and follows its evolution as well as the evolution of the mass distribution function consistently (Equations (15) and (16)). This method enables to treat the 2D (i.e., mass and porosity being dynamical) coagulation problems in a very efficient way. We have confirmed that our method well reproduces the results of previous full 2D Monte Carlo simulations with much fewer computational expense (Section 3).

2. We have presented a new collision model based on our numerical experiments on aggregates collisions (Section 4). A collision model refers to a set of definitions and formulae for the properties of porous aggregates, including a recipe for the porosity change upon a collision. As the first step, we have focused on “hit-and-stick” collisions, i.e., collisions involving no restructuring or fragmentation. In the numerical experiments, we have first considered successive collisions between aggregates of a fixed mass ratio, which we have referred as QBCCA. This allows to fill the gap between the classical BCCA and BPCA. Using the results of the \( N \)-body experiments on BCCA, BPCA, and QBCCA, we have constructed a recipe for the porosity change due to a general hit-and-stick collision (Equation (43)) as well as formulae for the aerodynamical and collisional cross sections. In a forthcoming paper, we will include the effects of collisional compression and fragmentation into our collision model.

3. To clarify the validity of our collision model and the difference from previous models, we have performed a couple of simple simulations on porous dust coagulation with the extended Smoluchowski method (Section 5). We considered two cases where the coagulation is driven by Brownian motion and differential drift, respectively. For both cases, the simulations using our model result in fractal aggregates of \( D \approx 2 \), which is consistent with the findings of previous full \( N \)-body and laboratory experiments (Kempf et al. 1999; Wurm & Blum 1998). By contrast, the simulations using the hit-and-stick model of OST07 result in much less porous aggregates. This is because this model underestimates the porosity increase upon unequal-sized collisions.

4. We have discovered that, when the coagulation is driven by differential drift, aggregates at the high-mass end of the mass distribution obey a flat density–mass relation, in marked contrast to aggregates of lower masses, which obey a fractal (i.e., power law) density–mass relation (Section 5.2). This is explained by the difference in the dominant growth modes: typical aggregates grow by colliding with similar ones, while the most massive aggregates grow by colliding with much smaller ones. As a consequence of this tendency, the massive aggregates can have a drift velocity (\( \times \) mass-to-area ratio) considerably higher than smaller ones. This finding may be crucially important in protoplanetary disks where the growth of slowly moving aggregates is suppressed due to the negative charging.

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