THE INFLUENCE OF MONOMER SHAPE ON AGGREGATE MORPHOLOGIES IN FIRST STAGE PROTOPLANETARY DEVELOPMENT

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Introduction: The coagulation of dust particles is an essential step in planetary formation. Planetesimals are believed to form via the collision of micron and submicron sized dust particles in the disk surrounding a newly formed protostar. Numerical models have been created to investigate the dynamics and properties of these dust aggregates [1-3]. Current models, however, usually analyze the dynamics of coagulation using spherical monomers. Further insight into fractal aggregation can be gained by studying the coagulation of non-spherical monomers such as ellipsoids.

A previous study modeled prolate ellipsoid and spherical monomers using particle-cluster and cluster-cluster aggregation methods (PCA and CCA respectively) [4], but concluded that the variation in morphology of resulting aggregates was too small for the monomer shape to be a significant factor in the overall structure or porosity of aggregates. However, the study did not include off-center impacts and rotational degrees of freedom in the parameter space. Additionally, the CCA model used the same aggregate as both target and impactor, while the PCA algorithm created artificially linear chains of monomers, by directing the incoming monomer to the nearest point on an aggregate. The goal of this work is to address these issues utilizing a more realistic aggregation method.

The morphology of aggregates built from ellipsoidal monomers, characterized by the compactness factor or fractal dimension, can be compared to that of aggregates built using spherical monomers. Analysis of the differences in morphology and porosity between these two populations will determine if spherical monomers are an acceptable approximation in all cases, or if monomers of other shapes are required to accurately model dusty systems in space environments.

Numerical Model: The numerical model used in this study, Aggregate Builder, simulates particle-cluster aggregation (PCA) and cluster-cluster aggregation (CCA) collisions and has been used in several previous studies modeling dust aggregation [1-3]. The code allows aggregates to be built with a variety of input parameters for the monomers such as radius, density, charge and magnetization.

The code was modified to allow for ellipsoidal monomers. This necessitated changes to the moments of inertia, used to calculate rotations of aggregates, as well as tracking the orientation of monomers within an aggregate. Charged or magnetized aggregates will also induce torques on the interacting grains. While these interactions were not included in this study, they also depend on the orientation of monomers within an aggregate and the moments of inertia and will be considered in future work.

Particles used in this model were of equal volume for both monomer shapes. A ratio of 3:1:1 was used for the ellipsoidal monomers giving an elongated, prolate shape. Radii used were $R = 2.885 \times 10^{-6}$ m for spherical monomers and a semi-major axis of $R = 6 \times 10^{-6}$ m for ellipsoidal monomers.

The model builds aggregates to large size initially using PCA collision. These aggregates are saved to a library and used to build larger aggregates through CCA. Initially, a single monomer (or aggregate) is placed at the center of the coordinate system and a second particle is shot towards its center of mass (COM) plus an offset. Monomers are assumed to stick at the point of contact and be held together via Van der Waals forces. Aggregates were built in several generations. First generation aggregates were built using PCA collisions up to around size N = 20. Second generation aggregates were built via CCA using first generation aggregates up to size N = 200. Third generation aggregates are built using CCA from both first and second generation aggregates up to N = 2000.

Results: The morphology of aggregate populations built using ellipsoidal monomers is compared to spherical monomers. Aggregates consisting of equal numbers of monomers are compared by their maximum radius (the radius of a sphere centered at the COM which just encloses the aggregate) in Figure 1.

Another measure of the morphology of aggregates is the porosity of the aggregate. The porosity is a direct measure of how much empty space is in an aggregate. The porosity is calculated via

$$P = 1 - \frac{V_s}{V_T}$$

where V_s is the sum of the volume of all of the monomers and V_T is the volume of a sphere with the maximum radius of an aggregate. Aggregate porosities from the two populations generated in this study are shown in Figure 2.

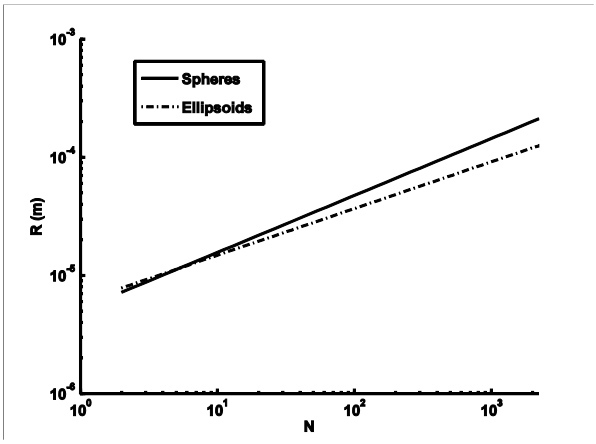

Figure 1. Maximum radius of aggregate versus number of monomers N. Spherical aggregates grow proportional to $R \propto N^{0.48}$, ellipsoidal aggregates grow proportional to $R \propto N^{0.39}$.

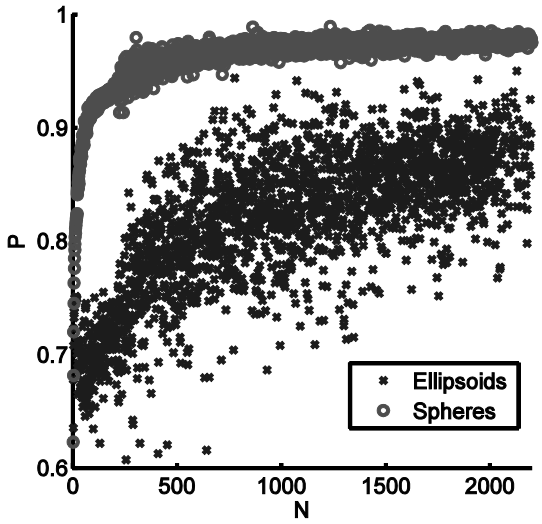

Figure 2. Average porosity of aggregates versus number of monomers N. Spherical monomers build very compact structures while ellipsoidal monomers result in a much wider range of possible porosities.

Two additional structural factors, the compactness factor and the friction time will also be analyzed in future work.

The compactness factor is a measure of the openness or fluffiness of an aggregate. Lower compactness factors correspond to more open structures, while high compactness factors correspond to more compact or spherical structures. The compactness factor is calculated from

$$\phi_\sigma = \frac{\sum r_i^3}{R_\sigma^3}$$

Here r_i corresponds to the radius of the i^{th} monomer within the aggregate for spheres, while for ellipsoids r_i^3 is defined as *abc*, where *a* is the semi-major axis and *b* and *c* are the semi-minor axes, and R_σ is the radius of the average projected cross section of the aggregate calculated for several random orientations.

The friction time is a measure of the effect of gas drag on the motion of a particle and dictates the dynamics of aggregates immersed in a gaseous environment, such as a protoplanetary disk. Large friction times may indicate that a particle is decoupled from the gas, leading to radial drift and vertical settling of particles. The friction time is given by

$$\tau_f = \frac{m}{\sigma} \frac{1}{\rho_g v_{th}}$$

Where *m* is the mass of the aggregate, σ is the average cross sectional area, ρ_g is the mass density and v_{th} is the mean thermal velocity.

Combining the results from these quantities allows a determination to be made as to whether the shape of dust monomers has a non-negligible effect on processes such as dust aggregation in a protoplanetary disk. The porosity and compactness factor are the most important measures of the structure and fluffiness of the aggregates. Not only do they give a measure of the overall structure of the aggregates, they yield an indication of the number of dissipation channels for aggregate energy during high energy collisions that might lead to compactification or fragmentation. A low number of dissipation channels would be correlated to a high porosity or low compactness factor.

References: [1] Matthews, L. S., T. W. Hyde (2008) *IEEE Trans. Plasma Sci.*, 36: 310-314 [2] Matthews, L. S., T. H. Hyde (2004) *IEEE Trans. Plasma Sci.*, 32: 586-593 [3] Perry, J., L. S. Matthews, T. W. Hyde (2010) *IEEE Trans. Plasma Sci*., 38: 792-797 [4] Bertini, I, P. J. Gutierrez, W. Sabolo (2009) *Astron. & Astrophys.*, 504: 625-633.