DUST GROWTH IN A PROTOPLANETARY DISK USING MOLECULAR DYNAMICS. Chuchu Xiang, Lorin S. Matthews, Augusto Carballido, and Truell W. Hyde. Center for Astrophysics, Space Physics and Engineering Research (CASPER), Baylor University, Waco, TX 76798, USA

Introduction: Coagulation of dust aggregates plays an important role in the formation of planets and is of key importance to the evolution of protoplanetary disks. This study compares the growth of neutral and charged dust in a turbulent protoplanetary disk, and analyzes the collision probabilities as a function of the physical characteristics of aggregate grains. For uncharged spherical grains, the coagulation probability (kernel) is a function of grain radius and relative velocity [1], while for aggregates, it is determined by additional factors such as mass and compactness factor. Another complication is that cosmic dust becomes charged in the radiative plasma environment, and the trajectories of colliding dust grains can be altered by the electrostatic force acting between them, affecting their coagulation probability [2]. It is difficult to develop an analytic kernel as a function of all of these parameters. Instead, we use a numerical method by collecting the statistics on detailed models of collisions and using regression analysis to find the probability of collision as well as the physical characteristics of the resulting aggregate. In this method, the simple kernel, which depends on radius and relative velocity, is used to choose potential colliding pairs, and the actual collision outcome is determined by a detailed collision model which takes into account the aggregate morphology, trajectory, orientation, and all forces acting on the colliding grains.

Coagulation Model: Coagulation was modeled for conditions in a turbulent protoplanetary disk at a distance of 3 AU. The initial dust population is silicate spheres with radii $0.5 \leqslant a \leqslant 10$ microns with a power law size distribution $n(a)da \propto a^{-3.5}\, da$ [2]. The hydrogen plasma environment had the same electron and ion temperature, $T_e = T_i = 900$ K. In the case of low dust density, a negligible percentage of the electrons reside on the dust grains, and the density of electrons and ions in the gas is set to be $n_e = n_i = 5\times 10^8\ m^{-3}$ [6]. The relative velocities between two interacting dust grains were set assuming the grains were coupled to turbulent eddies in a protoplanetary disk [9], with turbulent gas parameters provided by ATHENA [5], a grid-based code for astrophysical magnetohydrodynamics.

The temporal evolution of the dust population is determined by a Monte Carlo algorithm used to select colliding pairs. The fundamental postulate of this algorithm is that there exists a function $C_{ij}\ (m_i, m_j, r_i, r_j)$ which represents the probability that a given pair of particles with masses m_i, m_j and radii r_i, r_j will coagulate in the next unit time. In our case, $C_{ij} = \pi(r_i + r_j)^2 \Delta v_{ij}$ /V where $\pi(r_i + r_j)^2$, Δv_{ij} and V are the cross-sectional area, relative velocity of the two particles and the volume of the simulated region [1]. At time t, the probability that the next collision will occur in time interval $(t + \tau,\ t + \tau + d\tau)$, and involve particle i and j is

$$P(i,j,\tau) = C_{tot}\exp(-\,C_{tot}\tau)\times(C_i/C_{tot})\times(C_{ij}/C_i)$$

where the partial sum $C_i = \sum_{j=i+1}^{N} C_{ij}$ and the total sum $C_{tot} = \sum_{i=1}^{N-1} C_i$ [3]. The first term, $C_{tot}\exp(-\,C_{tot}\tau)$, is the probability that the next collision will occur between times $(t+\tau)$ and $(t+\tau+d\tau)$, independent of the colliding pair chosen. The time elapsed between two collisions, according to this probability, is given by $\tau = C_{tot}^{-1}\ln(1/r)$ with r a random number. The second and third terms represent the probabilities that the first chosen particle is i and the second chosen particle is j. In order to reduce the computational cost, the particles are binned into 100 groups by equivalent radius, and the average equivalent radius of each bin is used to calculate C_{ij}. The collision rate between groups i and j is $\widetilde{C_{ij}} = g_i g_j C_{ij}$, where g_i and g_j are the number of particles in the two groups [1]. When particles from group i and j collide, g_i and g_j are both decreased by 1, and g_{i+j} is increased by 1. A second particle is randomly chosen to be duplicated and g_r is increased by 1. The total number of particles in the simulation is thus constant and the spatial dust density is kept constant by adjusting the simulated volume.

As two aggregates approach each other, they can collide and stick at the point of contact, bounce, or miss. The prerequisite for colliding or bouncing is that at least one monomer in each aggregate overlap, with the outcome determined by the critical bouncing velocity calculated for the two aggregates [8]. The detailed interactions of the collision process are modeled by Aggregate Builder (AB) [2]. In each iteration, two particles are selected randomly from the library. One is placed with its center of mass at the origin as the target, and the other is shot towards its COM plus an offset. The initial distance between the two particles is set such that the potential energy due to the charge interactions is less than 60% of the initial kinetic energy. The relative velocity between the two aggregates is the sum of the Brownian velocity and the turbulent velocity. Upon a successful collision, the new aggregate is saved to the library. If the particles bounce or miss each other, no new particle is formed.

Results: Preliminary data are compared for the charged and neutral aggregates. Compactness factor is

defined as the ratio between the volume of all the constituent monomers and the volume of a sphere with radius equal to the equivalent radius, the radius of a circle with area equal to the projected cross-section averaged over many orientations [2]. Figure 1 shows that the compactness factor decreases as aggregates become larger, and neutral aggregates tend to be slightly more porous than charged ones. The porosity plays an important role in the collision probability because more open structures couple more strongly to the gas, which reduces the relative velocity between grains. Although open porous aggregates have a larger collision cross section, small aggregates can pass through the gaps of the extended arms [2]. This explains why the pairs including one small particle and one large particle tend to miss, as shown in Figure 2. Another important factor in the collision rate is the charge, as it affects both the porosity of aggregates as shown in Figure 1, and the collision rates as the charged dust experiences a repelling electrostatic force between aggregates, reducing their relative velocity [2]. This reduces the collision rate (Figure 3), but at the same time reduces their kinetic energy which results in lower bouncing rate. Therefore, the rate that particle pairs stick together is a balance between the two factors.

A linear regression and principal component analysis was used to determine that the compactness factor, equivalent radius, charge and relative velocity are the greatest contributors to the collision rate. The next step of this research will be to develop a heuristic model for the collision rate based on the data recorded from actual collisions. This new kernel will be used to simulate the evolution of a dust population over long time periods relevant to protoplanetary disk evolution.

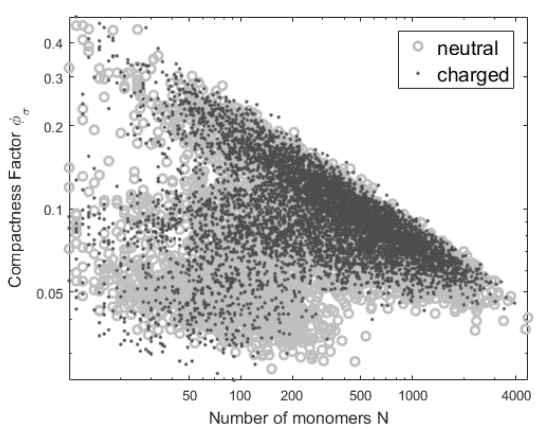

Figure 1. Compactness factor as a function of the number of monomers in each aggregate after ~80000 interactions. The aggregates grow more porous (i.e., a lower compactness factor) as the number of monomers increases.

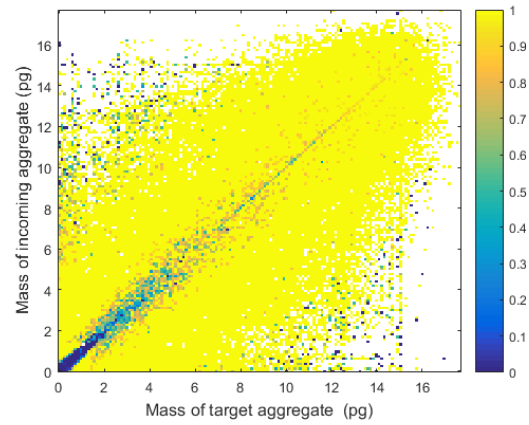

Figure 2. Collision probability as a function of the masses of the target and incoming charged particles. The collision rate of small charged aggregates is relatively low on the diagonal, as particles of similar sizes have low relative turbulent velocity.

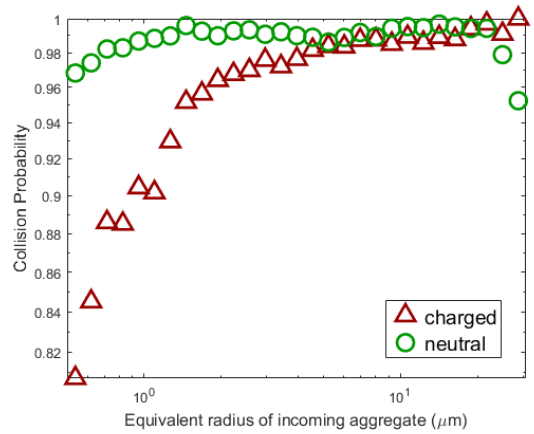

Figure 3. Collision probability as a function of the incoming aggregate's equivalent radius. Small charged particles have a lower collision probability than neutral ones, as they have relatively high charge to mass ratio, resulting in a high potential energy barrier.

References: [1] C. W. Ormel, M. Spaans, A. G. G. M. Tielens (2007) A&A 461, 215-232. [2] L. S. Matthews, V. Land, and T. W. Hyde (2012) ApJ 744 (1):8. [3] D. T. Gillespie (1975) AMS,1977-1989. [4] A. Carballido, J. N. Cuzzi, and R. C. Hogan (2010) MNRAS, 405 (4):2339–44. [5] A. Carballido, L. S. Matthews, and T. W. Hyde (2016) ApJ, 823 (2):80. [6] Q. Ma, L. S. Matthews, V. Land, and T. W. Hyde (2013) ApJ, 763 (2):77. [7] L. S. Matthews, D. A. Coleman, and T. W. Hyde (2016) IEEE Transactions on Plasma Science, 44 (4):519–24[8] A. Chokshi (1993) ApJ, 407:806-819. [9] C. W. Ormel (2008) ApJ, 679:1588–1610.