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A model of coagulation in dust clouds during grain charging

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Abstract

Initially uncharged grains in space and laboratory plasma environments become charged due to currents driven by potential differences in the dusty plasma. Certain macroscopic effects such as coagulation of smaller grains into larger ones or fluffy aggregates can be affected during this initial grain charging phase. The charging profiles of micron- and submicron-sized dust grains immersed in such plasma environments are strongly size- and temperature-dependent, and under certain conditions, the dust cloud can have various configurations of charged grains. Using a standard grain charging model along with a modified Barnes–Hut tree code for calculating grain dynamics, this paper examines the effect of including initial grain charging in coagulation of clouds of negative grains, positive grains, and a mixture of oppositely charged grains. The immediate application to coagulation during transient dusty plasma conditions is discussed.

Keywords: Dusty plasma; Coagulation in dust clouds; Grain charging

1. Introduction

Dust grains immersed in ambient plasma ("dusty plasma") become charged due to plasma ion and electron fluxes to grain surfaces. If the kinetic energy of the plasma electrons is sufficiently high, they can penetrate the grain surface and decelerate before becoming absorbed, thus imparting energy to electrons in the bulk of the grain, freeing them to possibly escape the grain surface as secondary electrons. The primary ion, primary electron and secondary electron currents can be significant for dust grains immersed in plasma in various space environments such as planetary rings and cometary tails (Goertz, 1989), astrophysical environments such as circumstellar and protoplanetary disks (Horányi and Goertz, 1990), laboratory environments of plasma etching of silicon wafers (Selwyn et al., 1989) and coulomb crystal formation (Thomas et al., 1994). If the dust is also immersed in a radiative environment, photoelectric and field emission currents can become significant as well.

Many models of collective charged dust effects employ calculations of grain charge at their asymptotic values; that is, the effect on dust cloud dynamics during grain charging from an initial to "steady-state" value is not considered. In space and laboratory phenomena which tend to have long time scales or ones not highly-dependent on grain charge, the variable nature of the grain charge may not present a significant problem. Often in these cases, the grain charge is able to "track" any plasma temperature or density change at the same rate. However, there are environments in which non-primary currents to the grain cause grain charging times to be significantly higher thus preventing the grain charge from tracking the transient effect with the same time scale. The present work considers the importance of

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grain charging on a given application of grain dynamics, that is, the coagulation of dust grains in a plasma. First, the grain charging model and a derivation of grain charging time is discussed. Subsequently the details of the method by which charging effects in a dusty plasma are modeled and the significance of coagulation in astrophysical environments is given. Finally, the model is applied to a representative problem and a discussion of the significance of the results is provided along with applications for treating transient effects in a future work.

2. Charging model

In this section we review the standard continuous charging model for currents to micron- and submicron-sized dust grains from the ambient plasma in which they are immersed. The discrete nature of the plasma particles is not considered; thus, the potentials calculated for the grain surface and plasma environment should be considered as average values. The charge on a dust grain Q_d at any specific time is strongly dependent on the plasma temperature kT_j number density n_j and velocity distribution as well as dust size distribution and motion. In moderate temperature plasmas ($kT_e > 15$ eV), the secondary-electron current caused by ambient electrons penetrating the surface of the grain, and thereby dislodging bulk electrons is significant. All three charging currents listed above are considered for the model presented.

The conditions for grain charge reaching equilibrium are the current conservation equation (Eq. (1)) and charge conservation equation (Eq. (2)) which are solved simultaneously for U and V:

$$J_{\text{tot}} = J_i(U,V) + J_e(U,V) + J_{se}(U,V,r) = 0 \tag{1}$$

and

$$Q_{dc}(U) + Q_p(V) = 0 \tag{2}$$

where J_{tot}, J_i, J_e and J_{se} are the total, primary ion, primary electron and secondary electron currents, respectively, to a grain of radius r (Bringol-Barge and Hyde, 2002). The quantities U and V are the dust surface potential (dust minus local cloud potential) and local cloud potential, respectively, following the notation of Havnes et al. (1990). The currents to the grain are driven due to the difference in dust and cloud potential, U. The quantities Q_{dc} and Q_p are the net charge gained by the dust cloud (localized collection of grains) and plasma, respectively. The dependence of the secondary electron current on grain radius is explicitly noted and can become a strong effect for submicron-sized grains through the secondary-electron yield for spherical grain geometry derived by Chow et al. (1993).

The normalized primary ion and electron currents are assumed to take the familiar form derived using OML theory

$$J_j = eZ_j n_j(V) \cdot \pi r^2 \cdot \sqrt{\frac{8kT_j}{\pi m_j}} \cdot \begin{cases} 1 - \frac{eZ_jU}{kT_j} & Z_jU \leqslant 0, \\ \exp\left(-\frac{eZ_jU}{kT_j}\right) & Z_jU \geqslant 0. \end{cases} \tag{3}$$

from Havnes et al. (1987), with j = i representing the primary ion current and j = e representing the primary electron current. The quantities Z_j, n_j, kT_j and m_j are the ion charge number, plasma number density, plasma temperature and ion mass, respectively, for plasma species j. The secondary electron current is taken from Chow et al. (1993) with added normalizing factors to be

$$J_{se} = en_e(V) \cdot \pi r^2 \cdot \sqrt{\frac{8kT_e}{\pi m_e}}(kT_e)^{-2} \exp\left(\frac{eU}{kT_e}\right) \cdot \int_0^\infty E\delta(E,r)\exp\left(-\frac{E}{kT_e}\right) dE, \quad U \leqslant 0, \tag{4}$$

$$J_{se} = en_e(V) \cdot \pi r^2 \cdot \sqrt{\frac{8kT_e}{\pi m_e}}(kT_e)^{-2} \exp\left(\frac{eU}{kT_e}\right) \times \exp\left(-\frac{eU}{kT_x}\right)\left(1 + \frac{eU}{kT_s}\right) \cdot \int_{eU}^\infty E\delta(E,r)\exp\left(-\frac{E}{kT_e}\right) dE, \quad U > 0$$

where kT_s is the thermal energy of the secondary electrons under the assumption they have a Maxwellian distribution leaving the grain, assumed to be 3 eV (Chow et al., 1993). The quantity $\delta(E,r)$ is the secondary-electron yield from a grain of radius r under bombardment from primary electrons of energy E. All grains are assumed to be insulating. The reader is referred to Chow et al. (1993) and Bringol-Barge and Hyde (2002) for details of the derivation of the secondary-electron yield and current.

The charge conservation equation, Eq. (2), with the assumption of a Maxwellian distribution of plasma ions and electrons, $n_j = n_{0j} \exp(-Z_j eV/kT_j)$, becomes

$$Z_i e n_{0i} \exp\left(-\frac{Z_i eV}{kT_i}\right) - en_{0e}\exp\left(\frac{eV}{kT_e}\right) + \overline{N}_d Q_d(U,r) = 0, \tag{5}$$

where V is the plasma cloud potential, n_{0j} is the plasma number density in the absence of dust, $\overline{N}_d$ is the modified dust number density, and Q_d is the charge on a dust grain of radius r.

An important simplifying assumption has been made at this point. In order to calculate the charge residing on an individual dust grain of radius r, we consider the presence of all other grains in the cloud to be a background of identically-sized grains of radius r and modified number density $\overline{N}_d$ (keeping the total cloud surface area constant). $\overline{N}_d$, is related to the actual dust density by $\overline{N}_d = N_d \cdot (4\pi r^2)^{-1}(\int 4\pi a^2 f(a) da)$. The limits of integration are from the minimum grain radius r_{min} to the maximum grain radius r_{max}, and $f(a) = a^{-s} da$ is the grain radius distribution function with S being the usual spectral parameter (typically between 0.9 and 4.5, depending on the cloud environment). This allows for faster calculation of grain charge while maintaining a high degree of accuracy. Through the two conservation equations, Eqs. (1) and (5), the equilibrium grain charge can be calculated. The following section deals with the additional important consideration of the time for grains to reach equilibrium.

3. Time scales and charging times

In any study of the effects created by changing dust charge and/or plasma parameters, it is important to consider dust grain charging times. The time required for a dust grain to reach its equilibrium value is usually defined as the time required for the grain to achieve one e-fold (63%) of its equilibrium value, following Cui and Goree (1994). To find the dust grain charging time, a first-order differential equation must be solved. Both the total current and charge conservation equations must be used as well as a calculation of charge from grain potential.

The relationship between the total current to the dust cloud and the charge on the dust cloud is given by $dQ_d/dt = J_{tot}$, where Q_d is the charge on the dust grain and J_{tot} is the total current to the dust grain. J_{tot} is thus comprised of the primary ion and electron currents as well as the radius-dependent secondary electron current. Assuming the charge on the dust grain can be calculated from the grain potential U (in volts) and grain radius r (in cm) through $Q_d = eUr/300$ with e being the electronic charge, the charging time is thus found to be

$$t_{ch} = \int_0^{t_{ch}} dt = \frac{r}{300}\int_0^{U_{eq}} \frac{dU}{J_{tot}(U,V)} = \frac{0.03306}{n_0(\text{cm}^{-3}) r_\mu \sqrt{T_{eV}}} \exp\left(-\frac{eV}{kT}\right)\int_0^{U_{eq}} \frac{dU}{J_{tot}(U,V)|_{norm}}, \tag{6}$$

where n_0 is in cm^{-3}, T_{eV} is the temperature in eV, the dust radius in microns is r_μ and J_{tot} is normalized to

$$en_0 \exp\left(\frac{eV}{kT}\right)\pi r^2 \sqrt{\frac{8kT_e}{\pi m_e}}. \tag{7}$$

For a 1 μm grain immersed in a hydrogen plasma with temperature 1 eV and ion and electron number density $n_0 = 1000$ cm^{-3}, the grain will achieve approximately 1750 electronic charges, and the calculated charging time is $t_{ch} = 1.46$ s. For the charging of grains in steady-state plasmas, the time-dependence of the grain potential and thus grain charge is exponentially asymptotic. Also to be noted is that, during the charging process (assuming the plasma parameters are not transient) the grain seems to take on only one sign of charge. That is, a grain that charges asymptotically to a positive value will take on positive values throughout the process. Fig. 1 shows the charging progression for a single 0.1 μm grain immersed in a $n_0 = 1000$ cm^{-3} hydrogen plasma for two different plasma temperatures. At a plasma temperature of 1 eV, the 0.1 μm grain will charge negatively while at a plasma temperature of 25 eV, the secondary electron current is high enough to cause the grain to charge to positive values.

It is interesting to see the effect of the radius-dependent secondary electron yield on charging times. Fig. 2 shows charging time as a function of temperature for an isolated 0.1 μm grain immersed in a plasma with number density 1000 cm^{-3}. The profile with the inclusion of secondary-electron current (curve A) is com-

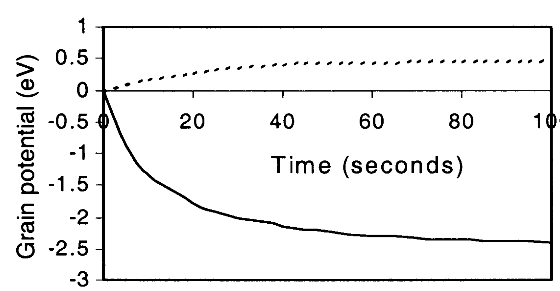

Fig. 1. Charge on a 0.1-μm grain as a function of time. The plasma density is 1000 cm^{-3}. The plasma temperature is 1 eV (solid line) or 25 eV (dotted line).

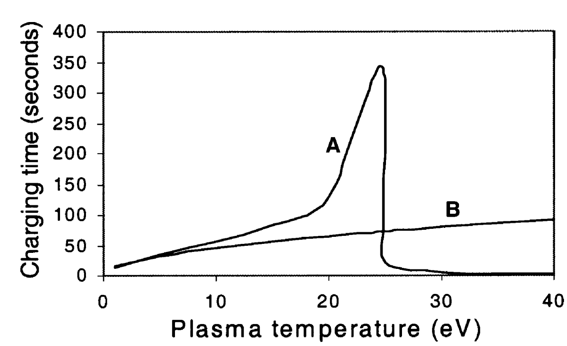

Fig. 2. Charging time for a 0.1-μm grain as a function of plasma temperature. Graph A includes secondary-electron yield while graph B does not.

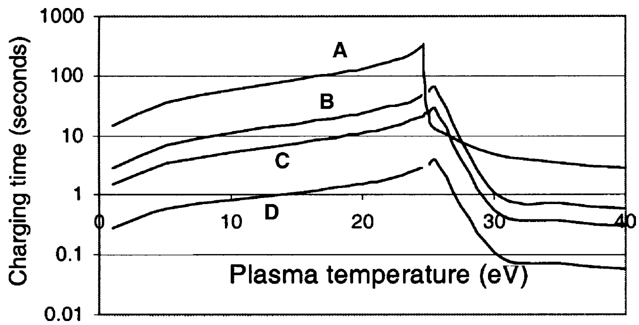

Fig. 3. Charging time as a function of temperature for: (a) 0.1 μm; (b) 0.5 μm; (c) 1.0 μm; (d) 5.0 μm grains. The plasma density is 1000 cm^{-3}.

pared with the exclusion of the secondary-electron current (curve B). Curve B shows the usual dependence of charging time with the square-root of the plasma temperature, $t_{ch} \propto \sqrt{kT_e}$ as shown by Cui and Goree (1994). The inclusion of the secondary-electron current which causes the grain to tend towards more positive values of charge, increases the charging time significantly. The maximum value of the charging time occurs at the plasma temperature at which the grain changes polarity; that is, when the grain can take on positive values. In Fig. 2, this "cross-over" temperature is around 25 eV. A comparison of charging times for grains in the range from 0.1 to 5 μm is shown in Fig. 3. The following general trends can be noted: submicron-sized grains have longer charging times than do micron-sized grains, and the temperatures at which grains become positive is lower for smaller grains. It should also be noted that charging times depend strongly on many other parameters, such as grain composition and dust cloud density. Therefore the above stated trends do not necessarily hold for all dusty plasma environments.

When considering grain charging processes during periods of time when there are physical changes occurring in the dusty plasma, apart from the plasma flux to the grain, it is important that the time scales involved be clearly understood. In order for the plasma velocity distribution to remain Maxwellian (or approximately Maxwellian), any changes in the plasma must take place on a time scale longer than the time for plasma thermalization. (This assumes, for the case of plasma depletion, that there is a mechanism present to insure the plasma remains thermalized.)

4. Updating grain charge

Under this assumption, the grain charge can be updated by considering the same first-order equation used to calculate the charging time. The differential equation is simply transformed into a difference equation in order to find the change in charge ΔQ during a change in time $\Delta t, \Delta Q = J_{tot}(U, V)\Delta t$, where J_{tot} is the value of the total current at each time step Δt during the charging process. At each step during the transient event, the appropriate J_{tot} calculated to find the change in grain charge.

The stepping time Δt is chosen so that the plasma has adequate time to thermalize (t_{therm}) during changes in plasma density or temperature, i.e. $\Delta t > t_{therm}$. The time for the plasma to thermalize (fill the gap in velocity space caused by the depletion of electrons and ions at plasma potential V) is taken to be the diffusion time for hydrogen ions and electrons and is taken from Havnes et al. (1987). Having detailed the theory for treating time-dependent charging in a dusty plasma, the numerical code used for grain dynamics will now be described.

5. Grain dynamics code

The numerical method for calculating intergrain forces is based on the box_tree code developed by Richardson (1993) to model large systems of particles interacting through gravity and modified by Matthews (1998) to include grain charge and electrostatic forces. The box_tree code is a hybrid of two computer algorithms, a box code which divides the system of particles into self-similar patches, and a tree code which provides a mechanism for fast calculation of interparticle forces using a multipole expansion. Each self-similar patch is assumed to have the same relative dust particle distribution with the boundary conditions met using ghost boxes (Richardson, 1993; Vasut and Hyde, 2001). The box_tree code has been successful in modeling a variety of physical systems ranging from charged dust in planetary rings (Matthews, 1998) to coulomb crystallization (Vasut and Hyde, 2001). The interested reader is directed to the papers listed above for details of the code.

The box_tree code updates the positions of the particles using the interparticle forces as a perturbation to the equations of motion. For a system of N charged dust particles in the absence of external electric and magnetic fields, the net force on the ith particle from all other particles is

$$F_{\mathrm{net},i} = \sum_{\substack{i=1 \\ i \neq j}}^{N} \frac{Q_i Q_j}{r_{ij}^2} \left(1 + \frac{r_{ij}}{\lambda_D}\right) \exp\left(-\frac{r_{ij}}{\lambda_D}\right), \tag{8}$$

with Q_i, Q_j being the charge on the ith and jth particles, respectively; r_{ij} is the distance between the centers of the ith and jth grains, and λ_D is the plasma Debye length, defined as $\lambda_D = 740(kT_e(eV)/n_e\,(cm^{-3}))^{1/2}$ cm from Grün et al. (1984). The particle masses, charges, number density and distribution, and velocities are supplied as input

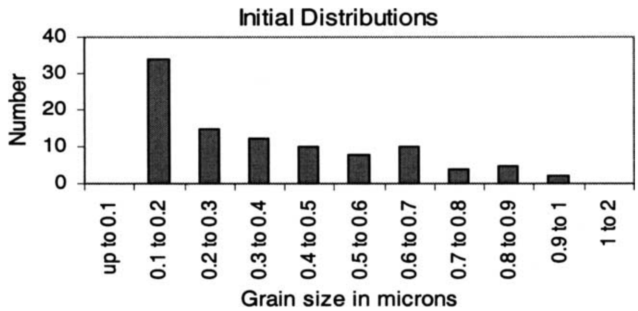

Fig. 4. Initial size distribution for all coagulation cases.

along with the Debye length of the ambient plasma. All these quantities can be updated and forces recalculated thus providing a code well-suited to examine grain coagulation during grain charging. We have assumed a dust-to-plasma number density ratio of $\overline{N}_{\rm d}/n_{0\rm e} \approx 10^{-3}$ which corresponds to a Debye length of 0.4 cm and an interparticle spacing of 0.01 cm. The densities used are greater than those found in astrophysical or space environments to decrease computational time. We do not expect the general trends to differ, only the coagulation rates. The specific problem of dust coagulation during charging is now discussed.

6. The coagulation problem

Dust grain coagulation is a process by which grains can stick together due to collisional interactions to form larger grains. Coagulation has long been considered an important growth process in various astrophysical and solar system environments such as the presolar nebula, protostellar and protoplanetary environments as well as cometary environments. Coagulation is considered to be one of the primary growth mechanisms for grains within the 0.1 μm to kilometer size range. For masses larger than kilometer size, the gravitational force be-

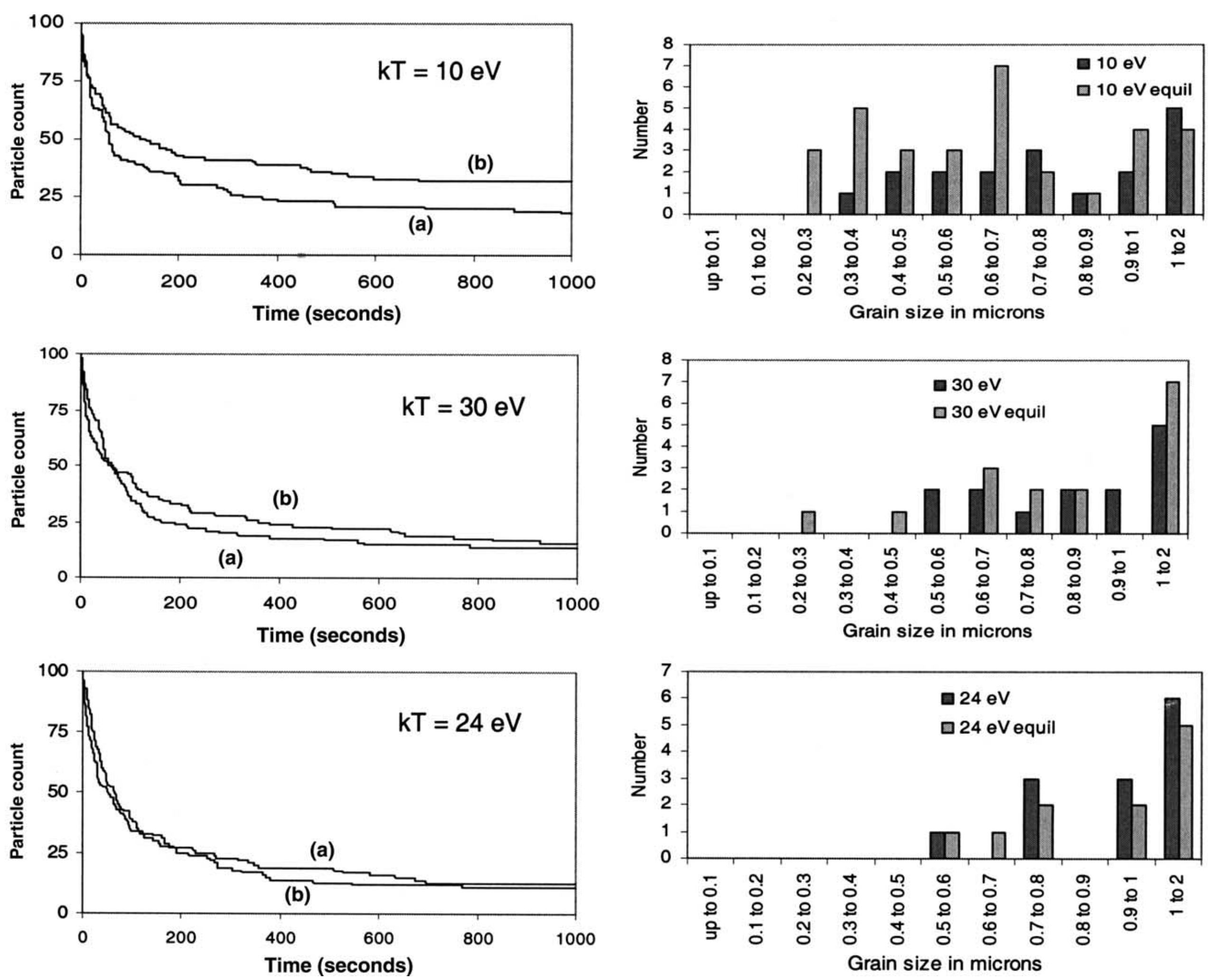

Fig. 5. Particle counts and final distributions (at $t = 1000$ s) during coagulation in dust clouds charged by 10 eV plasma (resulting in all negative grains), 30 eV plasma (resulting in all positive grains), and 24 eV plasma (resulting in oppositely charged grains). In case (a), all grains are assumed to initially be neutral. In case (b), all grains are assumed to remain at equilibrium values throughout coagulation process.

comes the dominant mechanism by which larger masses form. A full understanding of the physics of coagulation in the submicron to kilometer size regime has not been reached; however, there has been recent research which is improving our understanding of this growth process (Suttner et al., 1999).

In most early coagulation models, there was no assumption of charge residing on the dust even for micron and submicron grains. More recently, however, there have been several scenarios introduced that could possibly enhance coagulation through the presence of charged grains. The existence of grains with opposite charges in these environments is expected to increase the coagulation rate since the Coulomb force would then be attractive. Several simulations were run tracking the coagulation of 100 initially uncharged dust grains in a 0.01 cm^{-2} 2D box during charging under various plasma temperatures and an initial size distribution given in Fig. 4 (radial spectral parameter $S = 1.3$). All grains were assumed to have the same initial kinetic energy $kT_g = 10^{-4}$ eV. The resulting grain formed from the merging of two spherical grains was also assumed to be spherical. No ion or gas drag was included in the simulation. It should be noted that this model sets grain sticking coefficients to one, thereby not allowing for high-velocity collisions to fracture grains or cause elastic collisions. When a more realistic model for grain sticking is included, the above observations may not strictly be true.

7. Discussion

The three horizontal pairs of figures in Fig. 5 show the results of the coagulation model during charging of grains in 10, 30 and 24 eV plasma, respectively. Both the progression of coagulation during charging (compared to coagulation assuming grains initially have their equilibrium charge) and the final distribution of grains at $t = 1000$ s are presented. The three plasma temperatures are chosen due to the charge state of grains in the cloud. At $kT_e = 10$ eV, all grains are negative; at $kT_e = 30$ eV, all grains are positive; at $kT_e = 24$ eV, there exists both positive and negative grains in the cloud. Several qualitative results can be drawn by examination of the results. There seems to be the most significant difference in coagulation for the negative grains when initial charging is taken into consideration. In case (a) when the grains are initially uncharged, coagulation proceeds at a greater rate than in case (b) when all grains are assumed to take on their equilibrium value at $t = 0$. This general trend is also observed for the 30 eV case (all grains positive); however, due to the smaller magnitude of charge on positive grains in a cloud as compared to negative grains in cloud, the difference in coagulation rate is smaller. An interesting result is seen in the 24 eV case, with the cloud having both positive and negative grains. The coagulation rate is only slightly different than the equilibrium case, and in fact it proceeds at a slower rate. There is very little difference in the final distribution of grains at $t = 1000$ s. Therefore, from this initial qualitative study, we see that considering the initial charging of grains is most important in clouds with large magnitudes of charge, that is, in negatively-charged clouds.

We have presented the first results of a model which will be used in the future to study a variety of mechanisms, including plasma heating and plasma/dust injection by which coagulation rates can be significantly modified. A more detailed examination of coagulation rates according to grain size as well as specified size distributions and grain charging histories should also accompany such investigations in the future.

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