Astron. Astrophys. 340, 329–334 (1998)

ASTRONOMY AND ASTROPHYSICS

Free molecular gas drag on fluffy aggregates

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Received 29 July 1998 / Accepted 18 September 1998

Abstract. Dynamical behaviors of dust particles are governed by gas drag forces in a variety of environments of astrophysical interest, such as protoplanetary disks, upper planetary atmospheres or cometary coma. Monte Carlo (MC) and Quasi Monte Carlo (QMC) simulations have been performed to estimate the drag forces on fluffy aggregates in the free molecular limit, using two different models of molecule-surface interaction. The new computational scheme involves the concurrent evaluation of the rate of molecular collisions and the momentum transfer efficiency. It is found that the gas drag forces on a fluffy aggregate can be approximated by those on a sphere of equivalent area. The deviation from this approximation depends on the model of the molecule-surface interaction and on the size, structure, velocity and especially the orientation of the aggregate. The anisotropy of the drag force is mainly caused by the variation of the projected area when the velocity S, normalized by the mean thermal velocity of the gas, is larger than 1 and by multiple reflections of incident molecules when $S < 1$.

Key words: ISM: kinematics and dynamics – ISM: dust, extinction – solar system: formation – comets: general – molecular processes

1. Introduction

Both experimental (Wurm & Blum 1998, Praburam & Goree 1995) and theoretical (Richardson 1995, Ossenkopf 1993) studies have revealed that coagulation of solid particles generally produces fluffy aggregates. Analytical gas drag formulae in the free molecular region, which are available only for some simple shapes with convex geometry (Dahneke 1973), yield the well known result that the drag force is primarily determined by the number of collisions between the aggregate and the gas molecules, i.e., the geometrical cross section or the projected area of the aggregate. The larger projected area of fluffy aggregates, compared to that of a sphere of equivalent mass (hereafter a 'mass-equivalent sphere'), is supposed to significantly change their dynamical behavior in rarefied gaseous environments, such as protoplanetary disks (Weidenshilling & Cuzzi 1993; Hidaka & Nakagawa 1997) or upper planetary atmospheres (Berry 1989, Rannou et al. 1995). In particular, the ejection process of cometary grains from the nucleus is an interesting example. The terminal velocity $v(a,t)$ from the cometary coma depends on the time t and dust diameter a. Fulle et al. (e.g., 1997) found that the power index u of the size-dependence ($u = \frac{\partial v(a,t)}{\partial a}$) is generally smaller than the value expected from a classical model for spherical dust particles (Gustafson 1989). Their result, together with the appearance of chondritic porous interplanetary dust particles collected from the stratosphere, implies that cometary grains are aggregates of sub-micron grains with fluffy structures. Most of these studies, however, are based on the simple conjecture that the drag force on fluffy aggregates is proportional to their projected area equated to the equivalent sphere (Meakin & Donn 1988). The first attempt to validate this assumption for fractal dust aggregates was made by Meakin et al. (1989). They considered the Epstein regime, in which the dust velocities are much smaller than the mean thermal velocity of the ambient gas. Subsequently, Nakamura et al. (1994) studied the drag force on an aggregate moving much faster than the mean thermal velocity. Both studies still included the implicit assumption that the gas drag force can be expressed as the product of two independent factors:

1. the rate of molecular collisions,
2. the momentum transfer efficiency.

The former factor is supposedly proportional to the projected area and relative velocity of the aggregate and the gas density, while the latter depends on the surface structure of the aggregate and also on the model of the molecule-surface interaction. They independently estimated the two factors using the Monte Carlo (MC) method and simply combined them, neglecting any possible correlation. Although both results confirmed the conjecture that the gas drag force on fractal aggregates can be approximated by that on a sphere of equivalent projected area, the validity of the basic assumption has not been verified. Further, no quantitative study exists for the range of the relative velocities intermediate between the gas and aggregates.

In this paper we present a new numerical scheme that provides us with a direct estimate of the drag forces on fluffy aggregates for arbitrary relative velocities. In Sect. 2, we briefly describe the models for target aggregates and molecule-surface

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interaction. The validity of the computational procedure is established by comparisons with an analytical drag formula for a sphere and with previous numerical simulations of drag forces on two-touching spheres. The main results are given in Sect. 3. The last section discusses several implications of the results and their extension to the transition regime.

2. Computational procedures and the validity

First, two simple models of fractal aggregates are described, i.e., the Particle-Cluster Aggregate (PCA) and Cluster-Cluster Aggregate (CCA) models. In these models, aggregates are constructed by the ballistic coagulation of spherical constituent particles of equal radii. A PCA is generated by the successive attachment of constituent spherical particles to the seed cluster, whereas a CCA results from the collisions between clusters having the same number of constituent particles. The fractal dimension is nearly 3 for PCA, and 2 for CCA (see, e.g. Mukai et al. 1992). Secondly, we assume that the mean free path of gas molecules is much larger than the aggregate and the velocity distribution is Maxwellian. The interaction between the gas molecules and the surface of the aggregates is modeled using specular and cosine law diffuse reflection models (Meakin et al. 1989). We establish a Cartesian coordinate system, moving with the target aggregate, and neglect rotation. The origin of the coordinates is fixed at the center of mass of the aggregate, because its mass is much larger than that of an incident molecule. Incident molecules are successively fired into the virtual sphere enclosing the target aggregate with random impact parameters. By following the trajectory of an incident gas molecule, we calculate the final momentum transfer. The contribution of the molecule to the total drag force is estimated by calculating f, the momentum variation of the incident molecule weighted by its relative velocity. The resulting drag force is obtained from the arithmetic mean of f

$$E_N = \frac{1}{N_g}\sum_{k=1}^{N} f(\boldsymbol{x_k}) \tag{1}$$

where N_g is the number of incident molecules and $\boldsymbol{x_k}$ denotes the five dimensional vector specifying one incident molecule (i.e., two coordinates for the impact parameter and three velocity components). For the cosine diffuse reflection model, a standard Monte Carlo (MC) simulation is the only practical method to evaluate Eq. (1), since there is no one-to-one correspondence between an incident and emitted molecule because of the random nature of every reflection. In contrast, the momentum transfer of a molecule is determined uniquely for the specular reflection model. It is well known that the MC method is not optimal and that Quasi Monte Carlo (QMC) simulations give much faster convergence in these cases (Sarkar & Prasad 1987, Bratley & Fox 1988). Two sample calculations will be given below to demonstrate the capability of the computational procedures and the fast convergence of QMC.

For the specular reflection model, the gas drag force F_D on a spherical particle with a radius a is given by $F_D = 2C_D\pi a^2\rho v^2$

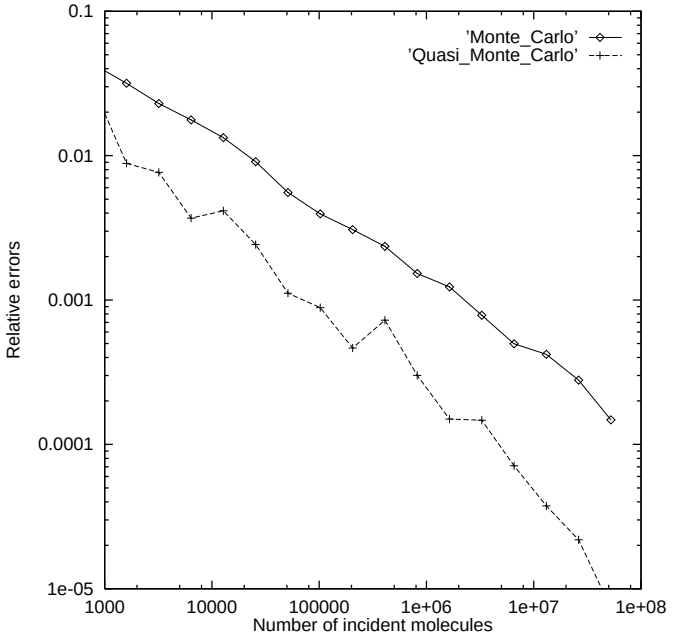

Fig. 1. Relative errors of our numerical calculations compared with the exact formula of Eq. (1) in the case of $S = 1$. The horizontal axis denotes the number of incident molecules N_g. Incident molecules are assumed to be reflected specularly on the surface. The average and standard deviation of 50 (5) different random (quasi-random) number sequences for MC (QMC) are plotted.

(Baines et al. 1965), where v is the velocity of the grain relative to the gas and ρ denotes the mass density of the gas. The drag coefficient, C_D, for the specular reflection is defined as

$$\frac{1}{2\sqrt{\pi}}\left\{\left(\frac{1}{S}+\frac{1}{2S^3}\right)\exp\left(-S^2\right) + \left(1+\frac{1}{S^2}-\frac{1}{4S^4}\right)\sqrt{\pi}\mathrm{erf}(S)\right\} \tag{2}$$

where S is a ratio of the velocity v relative to the mean thermal velocity of the gas v_g. This complicated formula simplifies in two limiting cases. When $S >> 1$, the drag coefficient approaches 1/2 and F_D is proportional to the square of the particle velocity. On the other hand, when $S << 1$, it reduces to the well-known Epstein law, i.e. $F_D = (4\pi/3)a^2\rho v v_g$.

Fig. 1 shows the relative error of our numerical simulations as a function of the number of incident molecules N_g. The curves indicate the difference between our numerical simulations and the exact formula of Eq. (2) for $S = 1$. For MC simulations, the asymptotic behavior when $N_g^{-1/2}$ is immediately confirmed. One can see that QMC converges much more rapidly and substantially outperforms MC. Next, our simulations for two touching spheres in the Epstein regime are compared with the previous work by Chan & Dahneke (1981). Table 1 indicates the values of the drag force on two-touching spheres for S = 0.1 normalized by the force on a single sphere. Two different directions, parallel and perpendicular to the line connecting the center of each sphere, are shown. Our calculations are in very good agreement with those by Chan & Dahneke. It can be concluded from Fig. 1

Table 1. The drag force on two-touching spheres for $S = 0.1$ normalized by that on a single sphere with same S.

Author	Parallel	Perpendicular
Chan & Dahneke	1.5478 ± 0.0047	2.08623 ± 0.00716
Present work	1.54397 ± 0.00057	2.09002 ± 0.00043

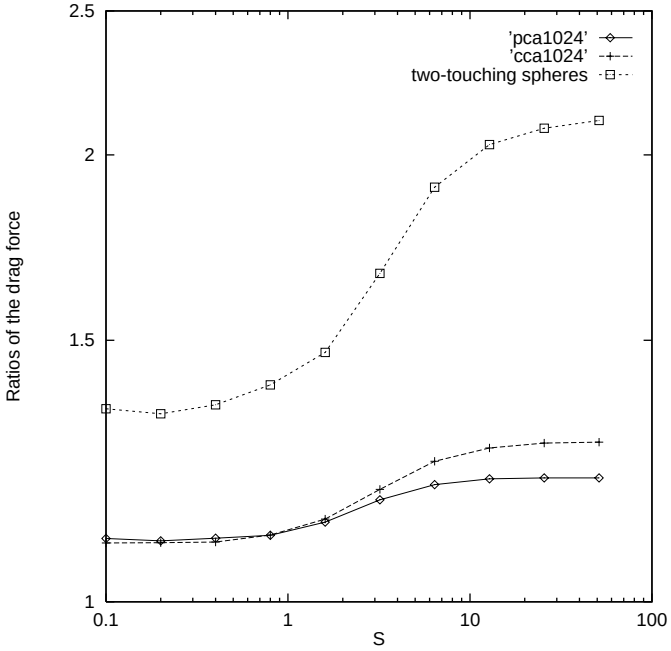

Fig. 2. The ratio of the drag force in the X direction compared to that in the Z direction (see text for their definitions). The targets are two-touching spheres and PCA/CCA with 1024 constituent particles. The horizontal axis denotes the target velocity normalized by the mean thermal velocity of the ambient gas molecules.

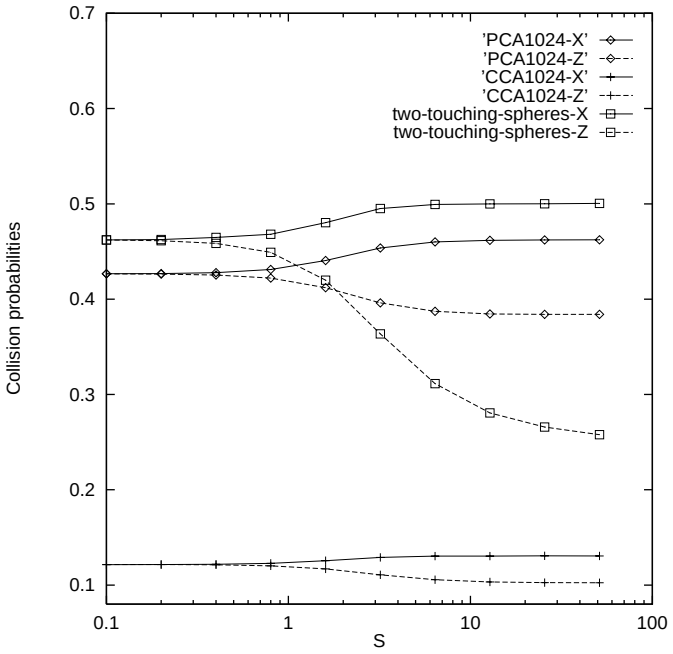

Fig. 3. The collision probability is defined as the fraction of incoming molecules that hit the target aggregate amongst all incident molecules fired into the virtual enclosing sphere with radius 'R_{max}'. For two-touching spheres, the radius of the virtual enclosing sphere is twice that of a constituent particle. Consequently, the collision probability goes to 0.5(0.25) in the large S limit for the X(Z) direction.

and Table 1 that we can obtain an accurate estimate of the drag force on fluffy aggregates for arbitrary values of S if we set N_g to a sufficiently large value. Since no analytic formula is available for irregularly shaped aggregates, we take a practical approach to confirm convergence (Fox 1986). A calculation is terminated when the estimated relative error $|E_{2N_g} - E_{N_g}|/E_{2N_g}$ becomes less than a certain tolerance called the convergence criterion. Further, we require that $|E_{2N_g} - E_{N_g/2}|/E_{2N_g}$ is also smaller than the convergence criterion to avoid accidental false convergence.

3. Results

Unlike a sphere, the shape of a fluffy aggregate is highly anisotropic. We select two directions of motion as extreme cases. One direction is along the axis of the aggregate with the maximum momentum of inertia (the X direction) and the other is the axis with the minimum momentum of inertia (the Z direction). These directions give, respectively, approximately the largest and the smallest projected area of the aggregate. The ratio of the drag force in the X direction compared to that in the Z direction is illustrated in Fig. 2. The targets are two-touching spheres and PCA/CCA consisting of 1024 constituent particles. It is apparent that the ratio is not unity for the whole range of S. As explained in the previous section, an incident molecule is launched along a ballistic trajectory randomly selected from all trajectories that pass within a distance R_{max} from the center of mass. Here R_{max} is the maximum radius of the cluster from the center of mass, i.e. the radius of the virtual enclosing sphere. Fig. 3 shows the collision probability of an incident molecule, defined as the fraction of impinging molecules that experienced at least one collision amongst all the incident molecules. The total number of collisions can be calculated from the collision probability and R_{max}. The "area equivalent sphere" of a fluffy aggregate is defined as a sphere with an area such that it experiences the same number of molecular collisions as the fluffy aggregate when the velocity and the ambient gas density are the same. It is found that the size of the "area equivalent sphere" bifurcates around $S \sim 1$ where the anisotropy of the incident molecule flux emerges. From Figs. 2 and 3, we immediately find that the dependence of the drag force on the direction of motion results from the shape anisotropy for $S >> 1$. However, what causes the variation of the drag force when $S << 1$ and the size of the "area equivalent sphere" is independent of the direction of motion? The distributions of f (see Eq. (1)) for two-touching spheres are shown in Figs. 4 and 5. The number of reflections of an incident molecule is found to alter the f distributions. The fraction of "back-scattered" molecules becomes larger in the X and smaller in the Z direction. This result means that the total

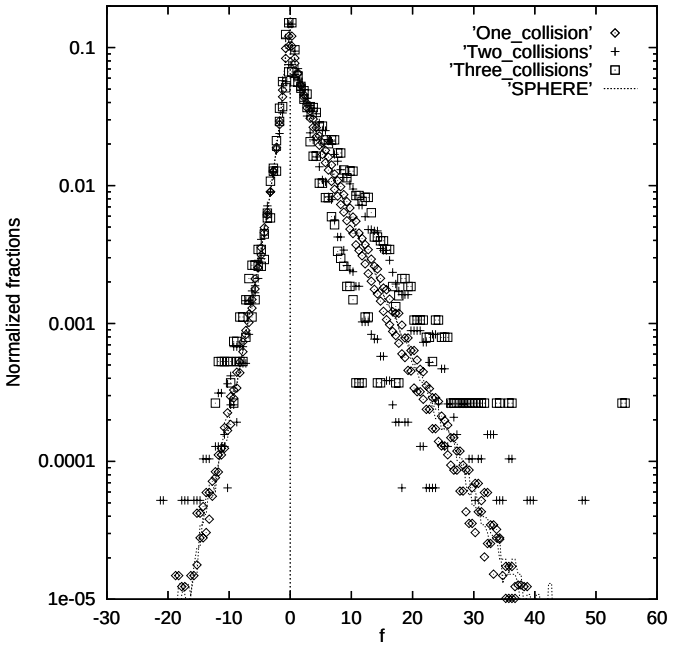

Fig. 4. The distribution of f for two-touching spheres moving in the X direction with S = 1. A positive value of f means that the molecule is scattered in the 'backward' direction and consequently transfers a large amount of momentum. The dotted line denotes the distribution of f for a sphere moving with S =1, for which multiple reflections are irrelevant.

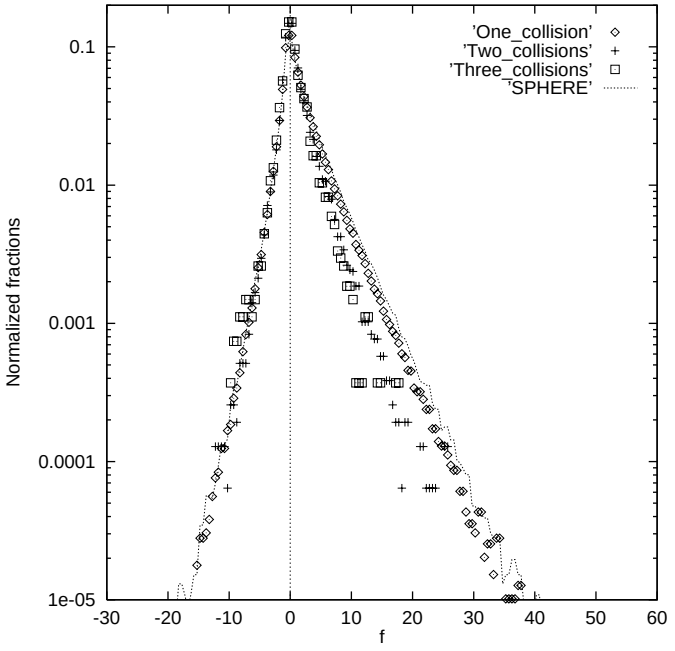

Fig. 5. Same as Fig. 4, but for the Z direction.

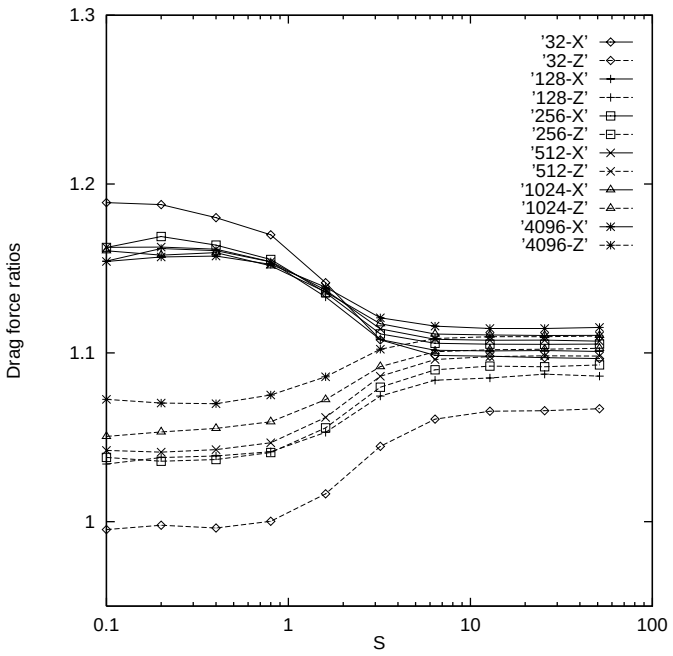

Fig. 6. The drag force ratios of PCA moving in the X and Z directions with the specular reflection model. The convergence criterion is 1 per cent. The data are averaged for 100 different aggregates in every size and velocity.

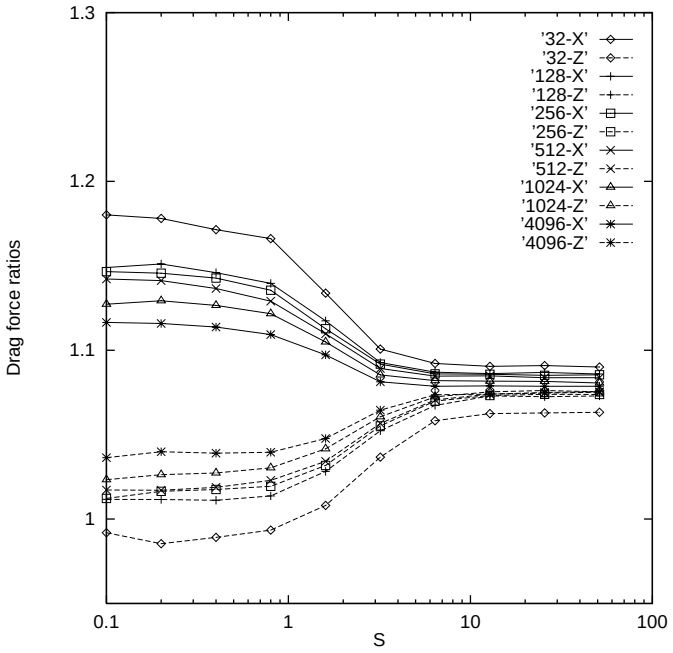

Fig. 7. Same as Fig. 6, but for CCA.

momentum transfer from gas molecules to the target is affected by multiple reflections.

In order to isolate the effect of multiple reflections, we employ the "drag force ratio", i.e. the ratio of the drag force on an aggregate to that on the "area equivalent sphere", with the specular reflection model. The drag force ratios of PCA and CCA are shown in Figs. 6 and 7 for the specular reflection model. The convergence criterion is 1 per cent over the whole range of S. For each size and velocity, we took the average of 100 different aggregates, so that the standard deviation roughly coincides with the convergence criterion. The values range from 1.0 to 1.2, depending on the number of constituent particles N, structure (PCA or CCA) and velocity S of the aggregates. When

$S < 1$, both PCA and CCA show an increase in the drag force ratio with increasing N for the Z direction and a decrease for the X direction. The limiting value of CCA for large N seems to converge to 1.08, while PCA does not reach a limit in this size range. Figs. 8 and 9 show the results for the diffuse reflection model. In contrast to specular reflection, diffuse reflection leads to a decrease for the Z direction with incresing N. The limiting value for large N cannot be reached, partly because the upper limit of N is smaller than that for the specular reflection model, for which we can use QMC with faster convergence.

Meakin et al. (1989) estimated the "momentum transfer efficiency" of CCA in the Epstein regime ($S << 1$). For the specular reflection model, the limiting value for $N \to \infty$ is 1.09, while diffuse reflection yields 1.27 without reaching a limiting value for N ≤ 1024. The rotational average of present calculations for CCA would find a consistent value for the specular reflection model, while the cosine diffuse reflection model gives somewhat higher values. On the other hand, in our previous work (Nakamura et al. 1994), we found that the "momentum transfer efficiency" is approximately 1.1 for CCA and 1.2 for PCA, in the large S limit for the specular reflection model. The large S limit of PCA is not consistent with the present calculations, even if we take into account uncertainties such as the convergence criterion and variance for different aggregates. These discrepancies may be attributed to the correlation between the momentum transfer efficiency and the collision rate, which has been neglected in the previous numerical studies. Blum et al. (1996) performed laboratory experiments to study the Brownian motion of micron-sized aggregates under micro- gravity conditions. Along with the diffusion coefficient D, the friction coefficient $f_{drag} = F_D/v$ has been estimated. In the Epstein regime, the drag force ratio can be related to the friction coefficient and the value becomes 1.11 $\pm$0.17. By considering an appropriate mixing of specular and diffuse reflection, we find acceptable agreement between the experiment and the present calculations.

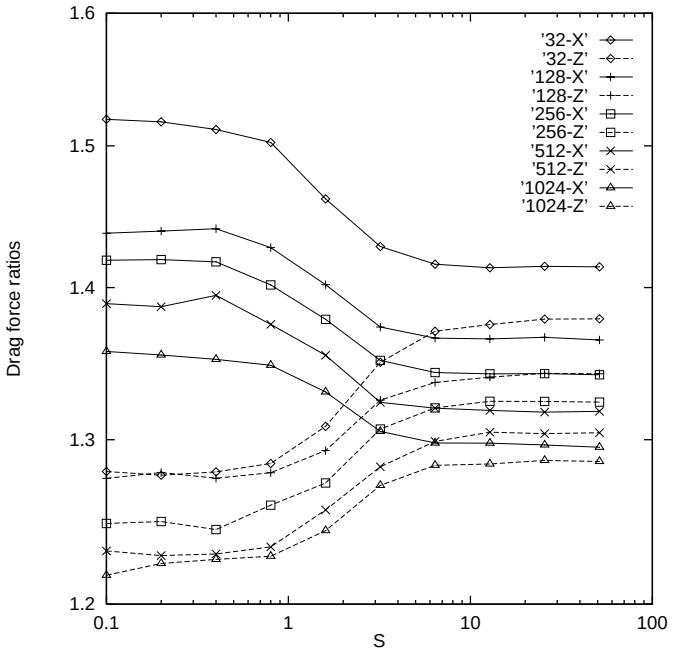

Fig. 8. Same as Fig. 6, but for the cosine diffuse reflection model.

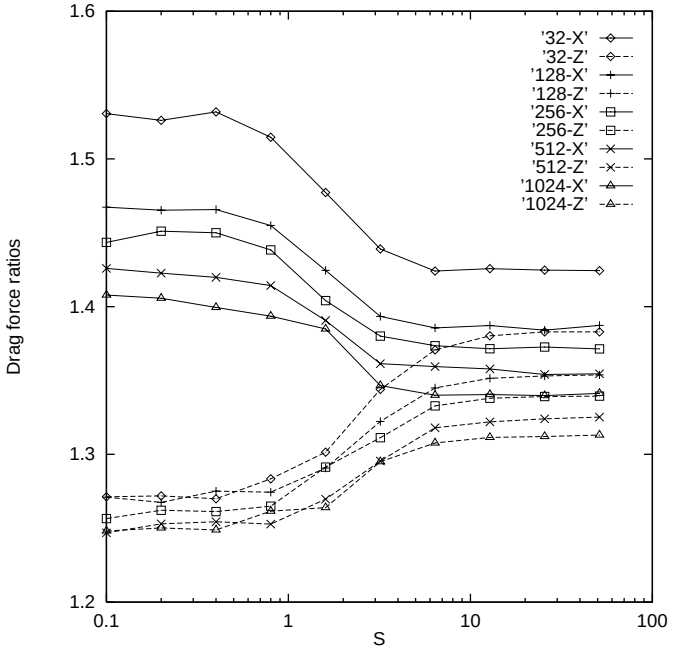

Fig. 9. Same as Fig. 8, but for CCA.

4. Conclusions and discussions

A new numerical scheme has been developed to investigate the interaction between fractal aggregates and gas molecules in the free molecular limit. The scheme allows for the irregular geometry of the aggregates and multiple reflections of the incoming molecules. The drag force is directly estimated over a wide range of relative velocities without separating the collision rate from the momentum transfer efficiency. The validity of the "area-equivalent sphere" approximation is explored quantitatively. In the limit of large N, we have found that the deviation from this approximation is less than 40 per cent. The larger projected area of fluffy aggregates has pronounced implications for dust growth in protoplanetary disks (Blum et al. 1996). Moreover, we have demonstrated that the surface irregularity of fluffy aggregates produces an anisotropic drag force even for S $<<$1. Although dust alignment has been supposed to be relevant only for supersonic motion (Gold 1952, Lazarian 1994), our results suggest that alignment may be possible even when the motion is subsonic. For example, the observed variability of polarization around cometary nuclei (Renard et al. 1996) may be explained by the alignment of dust aggregates in the inner coma. This subject will be investigated in our future work.

Finally, we mention the extension of our work to the transition regime, where the mean free path of the gas molecules is comparable to the size of an aggregate. For a spherical particle of diameter D and velocity v relative to the surrounding gas,

the drag force F in the transition regime is expressed by (e.g. Ying & Peters 1991)

$$F = \frac{3\pi\eta D v}{C(D)} \tag{3}$$

$$C(D) = 1 + Kn[\alpha + \beta exp(-\gamma/Kn)] \quad (Kn = \lambda/D) \tag{4}$$

where λ is the mean free path and η is the viscosity of the gas. The values of the coefficients α, β and γ can be found in Hutchins et al. (1995). Takata (1993) has given a theoretical basis to this formula by solving the Boltzmann equation numerically. Dahneke (1973) proposed an "adjusted sphere" generalization of Eq. (3) for non-spherical particles. In order to recover the correct limiting behavior, Eq. (3) is modified to become

$$F = \frac{3\pi\eta D_m v k_c}{C(D_a)} \tag{5}$$

where D_m denotes the diameter of a sphere of the same mass as the non-spherical particle and k_c is the dynamic shape factor in the continuum regime. The "adjusted diameter" D_a denotes the diameter of the area-equivalent sphere investigated in the present work. Used with values of k_c for fluffy aggregates (e.g. Rogak & Flagan 1992), our results have great utility in evaluating drag forces in the transition regime.

Acknowledgements. We greatly appreciate the critical reading of the original manuscript by Prof. T. Mukai and Dr. H. Ishimoto.

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