Computing the aerodynamic drag of fractal aggregates in free-molecular and transition regimes

Olga Stoyanovskaya$^{1,2}$, Anastasiya Suslenkova$^2$, Timur Kusnatdinov$^2$

$^1$Lavrentiev Institute of Hydrodynamics SB RAS, Ave. Lavrentieva, 15, Novosibirsk, 630090, Russia
$^2$Novosibirsk State University, Str. Pirogova, 1, Novosibirsk, 630090, Russia

E-mail: o.p.sklyar@gmail.com

Abstract.

For fine particles moving in the gas different regimes of aerodynamic drag are distinguished depending on their sizes and dust to gas relative velocities. In the Epstein or free-molecular regime, the drag force depends on the projected area or cross-section of the body, and in the Stokes or transition regime, on its linear size. Finding the linear size and the projected area for nonspherical particles is a non-trivial task. To describe the mobility of some type of nonspherical particles - fluffy aggregates, considered as a set of spheres - monomers, the value $D_f$ called fractal dimension is often used. For such aggregates with fixed fractal dimension $D_0$, several authors suggested the approximations of the linear size (called Smoluchowski radius $R_s$) and projected area $PA$ as a function of $N$ - the number of monomers in the aggregate. These authors validated their approximations on experimental data. On the other hand, new direct numerical simulation (DNS) data on mobility of fractal aggregates have been obtained recently. In the paper we constructed new functions $PA(D_f,N)$ and $R_s(D_f,N)$ interpolating available from the literature approximations of $PA(D_0,N)$ and $R_s(D_0,N)$ and minimizing the deviation from recent DNS data. These functions are designed for global simulations of protoplanetary discs dynamics and planet formation, but can be used in different applications.

1. Introduction

Mathematical modeling of the dynamics of gas and dust media or aerosol has a large number of applications. For some applications, it is essential to take into account the growth and fragmentation of dust particles as a result of collisions. It is known that collisions of fine particles in aerosol form fluffy aggregates (see fig.1 from [1]). The aerodynamic resistance of such aggregates significantly exceeds the aerodynamic resistance of compact objects - balls assembled from the same substance.

To simulate the aerodynamics of fluffy aggregates it is convenient to represent them as an ensemble of sticked spheres - monomers. Such a representation is fruitful due to the experimental fact that if an aggregate is assembled from monomers under certain and constant physical conditions, then its geometric or aerodynamic characteristics can be determined as a function of the number of monomers in the aggregate (see e.g. [5]). Since the same function for determining the geometric or aerodynamic characteristics corresponds to the different number of monomers in an aggregate, such objects are called self-similar or fractal. We will illustrate this idea by considering the computer model of assembling aggregates according to the Witten-Sander algorithm [11]. This algorithm allows to assemble a fractal aggregate on a plane, divided into

...
Figure 1. Panels a, b, c - morphology of flat fractal aggregates generated by the Witten-Sander algorithm. Panel d is the number of monomers in a ball of radius $r$, the center of which is the seed of the aggregate shown in panels a (red line), b (blue line), c (black line).

The algorithm works as follows. The monomer, which is the seed of the cluster, is placed on a cell in the center of the board, consisting of a large number of cells. Then a wandering monomer is added to the board. This monomer walks randomly in the plane to neighboring cells until it gets to the cell adjacent to the seed of the cluster. Once near the cluster, the wandering monomer sticks to it. After that, the next wandering monomer is added to the board, and so on. The Witten-Sander algorithm reproduces such a model of dust clusteres growth, in which monomers move under the same physical mechanism - Brownian motion of gas molecules - and collide with a cluster. It can be seen from the panels a-c in Fig.1 that due to the randomness of the walks of the wandering monomer, each run of the algorithm forms objects of different shapes. However, as follows from panel d of Fig.1, the volume concentration of monomers in the growing three objects obeys the same power law. Knowing this law, it is possible to determine the fractal dimension of the cluster $D_f$ (see e.g. [2]).
\[ D_1 = \frac{2}{3}, \quad PA(N) = 0.802(N - 1) + 1 \]
\[ D_2 = 1.78, \quad N^{0.92} \]
\[ D_3 = 1.8, \quad 0.478N + 0.5218N^{0.7697} \]
\[ D_4 = 1.95, \begin{cases} 15.2N^{2/3}\exp(-2.86/N^{0.096}), & N \leq 20, \\ 0.692N^{0.95}(1 + 0.301/\ln(N)), & N > 20. \end{cases} \]
\[ D_5 = 3, \quad N^{2/3} \]

\[ D_t \in [1.7; 2], \quad [1.624k_0^{-1/D_t}D_t^{-0.9}N^{0.47}]^2 \]

**Table 1.** Approximation of the projected area for different fractal dimensions of aggregates for the Epstein drag force computing. Here \( k_0 \) is a coefficient that determines the actual number of monomers of a fractal aggregate in a sphere of radius \( r \), that is, \( N = k_0r^{D_t} \).

\[ D_t = \frac{\ln N}{\ln(R_g/a)}, \quad (1) \]

where \( N \) is the number of monomers in the cluster, \( a \) is the radius of the monomer, \( R_g \) is the radius of the gyration of the cluster, which characterizes its linear size and is determined from the relation

\[ R_g = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (x_i - x_0)^2}, \quad (2) \]

where \( x_i \) is the radius vector of the center of the \( i \)-th monomer, \( x_0 = \sum_{i=1}^{N} x_i \) is the center of mass of the monomer.

The mechanism of aggregate growth, in which the dynamics of dust particles is provided by the Brownian motion of gas molecules, is called the DLA mechanism (Diffusion Limited Aggregation), if the growth is due to collisions "cluster-monomer" as in the Witten-Sander algorithm, and the DLCA mechanism (Diffusion Limited Cluster Aggregation) if growth is due to "cluster-cluster" collisions. It is known that in three-dimensional space aggregates growing according to the DLA mechanism have a fractal dimension \( D_t \approx 2.5 \), and according to the DLCA mechanism - \( D_t \approx 1.78 \) [1]. In addition, there are data on the fractal dimensions of aggregates growing by other mechanisms (for example, tables 1, 2 [12]).

Depending on the size and velocities of moving bodies, different modes of aerodynamic drag are distinguished. In the Epstein or free-molecular mode, the drag force depends on the projected...
area of the aggregate, and in the Stokes or transitional mode it depends on the linear size $R_s$, called the Smoluchowski radius or mobility radius. For spherical particles, projected area and the linear size are related by a simple relation $PA = \pi R_s^2$, however, for fractal aggregates such a relationship is a very rough approximation. To date, there are data on the effective projected area of aggregates of fractal dimension $D_f = 2/3$, 1.78, 1.8, 1.95, 3. These data were summarized in the functional dependence of $PA$ on the amount of monomers in the $N$ aggregate by the authors of [1], [8], [9], [10]. Known functional dependencies are presented in Table 1. Similar representations for $R_s$ are known for $D_f = 2/3$, 1.78, 3 and are given in Table 2.

It is clear that formation of real aggregates (formation of soot particles during combustion, sintering of fine particles in reactors with a fluidized bed of catalyst, accumulation of large bodies in astrophysical objects) is a result of both cluster-monomer and cluster-cluster collisions. Moreover, diffusion limited aggregation mechanism can be accompanied by convection-driven aggregation mechanism. Consequently, the fractal dimension of the resulting aggregates may vary in diapason from 2/3 (that corresponds to linear chains) to 3 (that corresponds to compact objects). To simulate the dynamics of objects of different fractal dimensions, we constructed approximations of $PA$ and $R_s$ as functions of two variables - the number of monomers $N$ and the fractal dimension $D_f$ of the aggregate.

The developed functions will be used primarily for modeling planet formation processes in circumstellar disks, where practically all known regimes of aerodynamic interaction of the solids with the gas take place. The simulation results [3] indicate that in a significant part of the disk, dust particles interact with gas in the Epstein regime. The next most common is the transitional regime. The development of models of global evolution of circumstellar disks goes in the direction of detailing models of dust dynamics. So recent works suggest that growing bodies in the circumstellar disk have a spherical shape [4] or constant fractal dimension. It can be expected that in the near future, new models free from these suggestions will be implemented and investigated.

2. Constructing functions for aerodynamic characteristics of fractal aggregates.

Problem statement and solution method

The aim of this work is to construct functions $PA(D_f, N)$, $R_s(D_f, N)$, where $D \in [2/3, 3]$ is a real number, $N \geq 1$ is a natural number, combining previously published data on the aerodynamic characteristics of three-dimensional fractal aggregates. Currently, there are two types of data. The first type is the functional dependences of the aerodynamic characteristics of aggregates with a fixed fractal dimension on an arbitrary number of monomers $N$. For example, Table 1 lists the projected area functions $PA_i(D_f = D_i, N)$, where $D_1 = 2/3$, $D_2 = 1.78$, $D_3 = 1.8$, $D_4 = 1.95$, and in Table 2 functions of Smoluchowski radius $R_{s,i}(D_f = d_j, N)$, where $d_1 = 2/3$, $d_2 = 1.78$. Such functional dependencies are well substantiated for $N \gg 1$. In the same tables, we have placed the definitions of $PA$ and $R_s$ for compact aggregates with $D_f = 3$. The second data type is the values $PA(D_f = D_i, N = N_j)$ and $R_s(D_f = D_i, N = N_j$) at a certain fractal dimension and a certain small amount of monomers. These data were obtained by the authors of [6, 7] by means of direct numerical simulation of collisions of aggregates with gas molecules. For the convenience we present these data in Table 3.

In order to obtain the desired functions of two variables, we built Lagrange interpolation polynomials in the variable $D_f$, using the known functional dependences on $N$ as the interpolation nodes, that is

$$PA(D_f, N) = \sum_{i=1}^{I} PA_i(N) l_i(D_f), \quad R_s(D_f, N) = \sum_{i=1}^{I} R_{s,i}(N) l_i(D_f),$$

(3)
Table 3. Projected area (third column) and Smoluchowski radius (fourth column) for aggregates with a fixed fractal dimension (first column) and the number of monomers (second column). The aggregates were generated on a computer by the authors of [6]. Aerodynamic characteristics were determined by the same authors by means of direct numerical simulation. The value of \( k_0 \) is defined in the caption of Table 1.

| \( D_f \), \( k_0 \) | \( N \) | \( PA \) | \( R_s \) |
|-------------|---|-----|-----|
| \( D_f = 2/3 \) | 2 | 1.846 | 1.392 |
| \( D_f = 2/3 \) | 3 | 2.693 | 1.718 |
| \( D_f = 2/3 \) | 5 | 4.386 | 2.319 |
| \( D_f = 2/3 \) | 10 | 8.617 | 3.594 |
| \( D_f = 2/3 \) | 20 | 17.081 | 5.793 |
| \( D_f = 1.78, k_0 = 1.3 \) | 5 | 4.228 | 2.193 |
| \( D_f = 1.78, k_0 = 1.3 \) | 10 | 7.870 | 3.033 |
| \( D_f = 1.78, k_0 = 1.3 \) | 20 | 14.998 | 4.357 |
| \( D_f = 2.5, k_0 = 1.5 \) | 5 | 3.839 | 1.975 |
| \( D_f = 2.5, k_0 = 1.5 \) | 10 | 6.718 | 2.586 |
| \( D_f = 2.5, k_0 = 1.5 \) | 20 | 11.856 | 3.437 |

Table 4. Comparison of candidate polynomials approximating the projected area with DNS data presented in Table 3. The first column is the interpolation nodes used to construct the Lagrange polynomial. The second column is the standard average squared deviation of the polynomial from the data.

| PA Interpolation Nodes | Average Squared Deviation from DNS data |
|------------------------|----------------------------------------|
| \( D_i = 2/3, 1.95, 3 \) | 0.6991822 |
| \( D_i = 2/3, 3 \) | 1.3793889 |
| \( D_i = 1.8, 3 \) | 1.6904368 |
| \( D_i = 1.78, 3 \) | 2.1197949 |

where \( l_i(D_f) = \prod_{j=1, j \neq i}^{D_f} \frac{D_f - D_j}{D_i - D_j} \) are basic Lagrange polynomials.

All elements \( D_i \) for \( PA \) and \( d_i \) for \( R_s \) or a sample from the corresponding sets were used as nodes for constructing the polynomials. The sample always contained a node corresponding to compact object. Thus, several candidate polynomials were built that approximate the desired functions \( PA \) and \( R_s \). The best approximations of \( PA \) and \( R_s \) were selected from the applicants, satisfying the criteria

- \( D_f \) monotonicity for \( N \geq 2 \) (the function must increase with increasing \( D_f \)),
- \( N \) monotonicity for \( 2/3 < D_f < 3 \) (the function must increase with increasing \( N \)),
- delivery of the minimum standard deviation from the data from Table 3.

2.1. Free-molecular drag mode. Projected area approximation

We considered Lagrange polynomials constructed on five (1 polynomial), four (4 polynomials), three (6 polynomials) and two (4 polynomials) interpolation nodes as contenders for the best approximation of the projected area. Fig. 2 compares all the contenders with the DNS results from the Table 3. The dots show the DNS results, solid lines - the contender polynomials. Red colour is used for \( D_f = 2/3 \), green for \( D_f = 1.78 \), blue for \( D_f = 2.5 \). It is immediately clear that only the polynomials shown in Panels 6, 8, 9, 11-14 can satisfy the \( D_f \) monotonicity criterion. On the contrary, in Panel 1 we can see that \( PA(2.5, 5) > PA(2/3, 5) \), so \( D_f \) monotonicity criterion
Figure 2. Projected area as a function of the number of monomers $N$ and the fractal dimension of the aggregates $D_f$. Points - data from Table 3, solid lines - approximating functions: candidate polynomials constructed on different sets of nodes. Red color shows data for fractal dimension $D_f = 2/3$, green - for $D_f = 1.78$, blue - for $D_f = 2.5$. 
is violated. At the same time, the polynomials presented in Panels 6, 9, 11 approximate the experimental data too roughly for \( D_t = 2/3 \) and \( D_t = 2.5 \) and therefore immediately excluded from the list of applicants. In order to choose the best approximation in the sense of criterion 3 from the remaining polynomials, we calculated the average squared deviation from the DNS data and presented the result in Table 4. Thus, it turned out that from the number of Lagrange polynomials, to approximate the projected area of fractal aggregates, the optimal one is a polynomial built using three nodes \( D_t = 2/3, 1.95, 3 \) and having the form:

\[
\begin{cases}
PA(D_t, 1) = 1; \\
PA(D_t, N) = 0.3340(D_t - 1.95)(D_t - 3)(0.802(N - 1) + 1) + \\
+0.4082(D_t - 2/3)(D_t - 1.95)N^{2/3} - \\
11.2801(D_t - 2/3)(D_t - 3)(N^{2/3} \exp(-2.86/N^{0.996})), \quad 2 \leq N \leq 20, \\
-0.5135(D_t - 2/3)(D_t - 3)(N^{0.95}(1 + 0.301/\ln(N))), \quad N > 20.
\end{cases}
\]  

(4)

The resulting approximation of the projected area (4) is a complex functional dependence on \( D_t \) and \( N \). To ensure the monotonicity of \( PA \) with respect to \( D_t \) for a fixed \( N \), a graphical method was used. In particular, the \( D_t - PA \) graphs were considered for \( N = 10, 20, 50, 100, 1000, 10000 \), on each of which the function turned out to be monotonic. The monotonicity of \( PA \) with respect to \( N \) for a fixed \( D_t \) is straightforward.

Due to the complexity of the resulting function its implementation in numerical simulations will require large number of arithmetic operations. To justify extra numerical costs let us compare the accuracy of (4) with simpler counterparts

\[
PA(D_t, N) = N^{2/D_t},
\]  

(5)

and

\[
PA(D_t, N) = \left[1.624k_0^{-1/D_t}D_t^{-0.9}N^{0.47}\right]^2.
\]  

(6)

The (5) function is a basic parameterization of projected area. The function (6) is proposed in [13] and validated for \( D_t \in [1.7; 2] \), \( k_0 \in [0.7; 2] \). Both functions have \( N \) and \( D_t \) monotonicity.

The results of comparison of the approximation with the DNS data are shown in Fig. 3, where the function we found (4) is presented on the left panel, on the central panel - (6), on the right - (5). It can be seen that the functions (6) and (5) are significantly less accurate than (4) when describing the projected area of aggregates with few monomers.

2.2. Transient or linear Stokes drag mode. Smoluchowski radius approximation

As contenders for the best approximation of the Smoluchowski radius, we considered Lagrange polynomials constructed on two (two polynomials) and three (one polynomial) interpolation nodes. By analogy with the previous case, we presented the applicants in Fig. 4 and compared the functions with the DNS data from Table 3. From Fig. 4 it can be seen that the polynomial built on 3 nodes does not satisfy the \( D_t \) monotonicity criterion, and the polynomial built on the nodes \( d_2 = 1.78, \ d_3 = 3 \) turns out to be closer to the DNS results than the polynomial built on the nodes \( d_1 = 2/3, \ d_3 = 3 \). This conclusion confirms the calculation of the average squared deviation of polynomials from DNS data, which turns out to be 0.3660181 and 0.7238013, respectively.

Thus, from the number of Lagrange polynomials constructed on the nodes \( d_i \) from Table 2, the optimal approximation of the Smoluchowski radius turned out to be a function...
**Figure 3.** Projected area as a function of the number of monomers $N$ and the fractal dimension of the aggregates $D_f$. Points - data from Table 3, solid lines - approximating functions: left panel - approximation proposed by us (4); central panel - approximation (6) suggested in [13]; right panel - basic parameterization (ref eq: PA_simple). Red color - data for fractal dimension $D_f = 2/3$, green - for $D_f = 1.78$, blue - for $D_f = 2.5$. On the central panel, the lines corresponding to $D_f = 2/3$ and $D_f = 2.5$ are shown as dashed lines, since the approximation (6) is validated only for $D_f \in [1.7; 2]$. The dashed lines were drawn using the values of $k_0$ from Table 3.

**Figure 4.** Smoluchowski radius as a function of the number of monomers $N$ and the fractal dimension of aggregates $D_f$. Points are data from Table 3, solid lines are approximating functions. The lower right panel is the standard parameterization (8), the rest of the panels are candidate polynomials constructed on a different set of nodes. Red color shows the results for $D_f = 2/3$, green - for $D_f = 1.78$, blue for $D_f = 2.5$. 
\[ R_s(D_f, N) = \begin{cases} 
0.8197 \left( (3 - D_f)N^{0.46} + (D_f - 1.78)N^{1/3} \right), & N \leq 100, \\
0.5328(3 - D_f)N^{0.56} + 0.8197(D_f - 1.78)N^{1/3}, & N > 100. 
\end{cases} \quad (7) \]

We compared the function (7) with the basic parameterization of the Smoluchowski radius
\[ R_s(D_f, N) = N^{1/D_f}. \quad (8) \]

From the right panels in Fig. 4 it follows that the function (7) is significantly accurate than (8) on aggregates with few monomers.

3. Discussion and conclusions
To simulate the dynamics of aerosol, we constructed functions that approximate the aerodynamic characteristics of nonspherical particles - the projected area or cross-section used to calculate the drag force in the free-molecular (Epstein) mode, and the Smoluchowsky radius used to calculate the drag force in transient (Stokes) mode. The non-spherical particles considered in this work are fractal aggregates from sticked spheres. The Smoluchowsky radius (7) and the projected area (4) of such aggregates are defined as functions of the fractal dimension and the number of spheres (monomers). It is shown that for aggregates with few monomers, the new functions much better approximate the recent DNS data [6] than the previously used approximations. On the other hand, calculating the new functions (7) and (4) requires more arithmetic operations.

Acknowledgments
This study was founded by budget project of Lavrentiev Institute of Hydrodynamics SB RAS.

References
[1] C. M. Sorensen (2011), Aerosol Science and Technology, DOI: 10.1080/02786826.2011.560909.
[2] A.V.Kolesnichenko, M.Ya.Marov (2014) Modeling of formation processes of fractal dust clusters as building blocks for protoplanetesimal in Solar protoplanet nebulae. Preprint of Keldysh Institute of Applied Mechanics, pp 44 [in Russian].
[3] Stoyanovskaya, O. P., Okladnikov, F. A., Vorobyov, E. I., Pavlyuchenkov, Y. N., Akimkin, V. V. (2020) Simulations of Dynamical Gas-Dust Circumstellar Disks: Going Beyond the Epstein Regime. Astronomy Reports 64, 107.
[4] Vorobyov, E. I., Akimkin, V., Stoyanovskaya, O., Pavlyuchenkov, Y., Liu, H. B. (2018) Early evolution of viscous and self-gravitating circumstellar disks with a dust component. Astronomy and Astrophysics 614, A98.
[5] Wurm, G., Blum, J. (2000) An Experimental Study on the Structure of Cosmic Dust Aggregates and Their Alignment by Motion Relative to Gas. The Astrophysical Journal 529, L57.
[6] R. Gopalakrishnan, C. J. Hogan, T. Thajudeen (2011), The Journal of Chemical Physics, 135(5): http://dx.doi.org/10.1063/1.3617251.
[7] T. Thajudeen , R. Gopalakrishnan and C. J. Hogan Jr. (2012), Aerosol Science and Technology, 46(11):1174-1186, https://doi.org/10.1080/02786826.2012.703353.
[8] Ossenkopf V. 1993. Dust coagulation in dense molecular clouds: the formation of fluffy aggregates. Astron. Astrophis. 280, 617-646 (1993) http://articles.adsabs.harvard.edu/pdf/1993A&A...280..617O.
[9] Chan, P. and Dahneke, B. 1981. Free-Molecule Drag on Straight Chains of Uniform Spheres. J. Appl. Phys., 52: 3106-3110.
[10] Meakin, P., Donn, B. and Mulholland, G. W. 1989. Collisions Between Point Mass and Fractal Aggregates. Langmuir, 5: 510–518.
[11] T. A. Witten, Jr. and I. M. Sander 1981. Diffusion-Limited Aggregation, a Kinetic Critical Phenomenon. PHYSICAL REVIEW LETTERS, 47(19)
[12] B. M. Smirnov 1986. Fractal Clusters. Success of science in physics, 149(2): 54-138 [in Russian].
[13] Mackowski, D. W. (2006). Monte Carlo Simulation of Hydrodynamic Drag and Thermophoresis of Fractal Aggregates of Spheres in the Free-Molecular Flow Regime, J. Aerosol Sci. 37:242-259.