EXPERIMENTAL AND THEORETICAL MEASUREMENT OF THE AERODYNAMIC DIAMETER OF IRREGULAR SHAPED PARTICLES

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ABSTRACT

A theoretical technique has been developed and verified experimentally for determining the aerodynamic diameter of irregular shaped particles. The aerodynamic diameter of a particle is a very important parameter for determining where that particle deposits in the respiratory tract. Many instruments, such as impactors and cyclones, will determine the aerodynamic size distributions of aerosol particles but few analyze the particles individually. The theoretical approach of our technique is to solve, by use of high speed computers, the three-dimensional Navier-Stokes equations to obtain the flow field around an irregular shaped particle of any contour. The computer program will then determine the drag on the particle, and thus the aerodynamic diameter of the particle can be calculated. The experimental approach has been to pass the particles through a centrifuge and collect the particles upon a collection foil. The position of a particle on the foil is an indication of its aerodynamic diameter. These particles were then shadowed in two orthogonal directions and inspected under an scanning electron microscope (SEM). The top view of the particle in the SEM plus the views of the two orthogonal shadows allows one to determine the three-dimensional shape of the particle. Studies have been performed on silica, coal and talc particles with aerodynamic diameters in the 1 to 4 µm size range. The three-dimensional shape, as is determined from SEM analysis, was used in the theoretical computer program and the results compared. It was found that in most cases the agreement between the experimentally and theoretically determined aerodynamic diameters was within 5%.

INTRODUCTION

The equivalent aerodynamic diameter (EAD) of a particle, defined as the diameter of a unit density sphere with the same falling speed as the particle in question, is an important size measurement of the particle. This is especially true when attempting to predict where particles may deposit in the respirator tract. Therefore, EAD is an important parameter when considering respiratory diseases caused by particles, such as coal workers pneumoconiosis (CWP).

Many instruments will measure the EAD size distribution of the aerosol particles, but few analyze the particles individually. Impactors, cyclones and virtual impactors normally collect particles upon substrates or filters which are then analyzed gravimetrically to determine the mass concentration of the particles in that size classification. The EAD of particles can be measured on an individual basis with centrifuges, inertial spectrometers and the TSI Aerodynamic Particle Sizer (APS). Centrifuges are most ideally applicable for studying individual particles as the particles are deposited, on long removable foils, at locations dependent upon their EAD.

The theoretical approach to determining the EAD of a particle has been primarily limited to regular shaped particles of symmetry to which analytical solutions of the flow field equations for air flowing around the particles can be applied. However, if the particle is irregular in shape, these analytical approaches do not apply and the EAD is very difficult to calculate. One technique that can be applied to determine the flow field around an irregular shaped particle is the numerical solution of the Navier-Stokes equations. In aerosol technology applications, this technique has been primarily used to determine the flow field through instruments. In most of these problems, the Navier-Stokes equations have only been expressed in two dimensions. However, to be able to describe the flow around any arbitrary irregular shaped particle, the Navier-Stokes equations must be solved in three dimensions.

The object of this paper is to apply the numerical solution of the three-dimensional Navier-Stokes equations to the flow around any irregular shaped particle and demonstrate that the aerodynamic diameter, so calculated, agrees with that determined experimentally in a centrifuge. Studies have been performed on silica, coal and talc particles with aerodynamic diameters in the 1 to 4 µm size range.

The shape of the particles used in the numerical solution of the flow field are defined by scanning electron microscopic (SEM) analysis of the particles collected on the foil in the centrifuge. An important discovery was made in the process of determining the three-dimensional shape of a particle in the SEM. It was found that the two-dimensional view of a particle is not sufficient to fully describe the shape of the particle. To fully describe the particle, it is necessary to shadow the particle with a film in two orthogonal directions. These two shadows, along with the plane view of the particle, can then provide a reasonable indication of the particle shape.

NUMERICAL ANALYSIS TECHNIQUE

Numerical analysis of the Navier-Stokes equations has been used extensively in our laboratory to obtain information on flow fields through aerosol analyzing instruments.[1-3] Although several techniques have been used to solve the Navier-Stokes equations, they are all basically the same in that the finite difference form of the equation is expressed in terms of the stream function and vorticity, or in terms of the velocity vector components and the pressure. A grid is placed over the area of interest and the finite difference equations are solved at the node points (intersection of the grid lines) of the grid. The solution is achieved by an iterative relaxation procedure that determines the value of the stream function and vorticity or the velocity vector components and the pressure at each node point. Since numerical solution techniques have been used extensively and many cases reported in the literature,[4,5] the techniques will not be described in detail here.

The particular numerical solution technique used in the work described here is that described by Patankar.[4] The reader is referred to his textbook for details of the technique. This technique solves for the velocity vector components and the pressure at the node points rather than the stream function and vorticity. However, once the velocity vectors and pressure are known, the stream function and vorticity can be calculated, if desired. The stream function is often calculated so that the stream lines (lines of constant stream function) can be shown to provide a clearer understanding of the nature of the flow fields.

Most of the work utilizing finite difference solutions to the Navier-Stokes equations has been in two dimensions. However, three-dimensional solutions can be obtained[6] and must be used when analyzing the flow around random irregular shaped particles. The solution technique is exactly as has been described by the two-dimensional analysis of Patankar, with the addition of the third direction. However, the computer program is substantially larger and the solution time much longer.

The fluid drag acting on the particle and the EAD can be computed from the numerically determined flow field surrounding the particle. Based on the calculated flow field, the fluid drag on the particle surface can be calculated by integrating the fluid stresses over the surface of the particle. The drag force on a particle will be the sum of both the pressure forces on the particle and the shear forces resulting from the fluid flowing past the surface of the particle. Once the drag force is equated to the gravitational force acting on a particle, the EAD is computed based on its basic definition. Since the aerodynamic diameter is defined as the diameter of a unit density sphere which falls at the same speed as the particle in question, the problem reduces to one of determining the falling speed of a particle. This problem further reduces to one of determining at what speed the drag force is equal to the gravitational force on particle, for these are the conditions which must exist when the particle is falling in equilibrium at its terminal settling speed.

Verification of Numerical Technique on Regular Shaped Particles

Since two-and three-dimensional computer algorithms had not previously been applied to determining the flow around particles, the first step was to verify the programs on regular shaped particles where analytical solutions for the flow fields exist. The algorithms were therefore applied to particles that are symmetric in shape such as spheres, cylinders and disks. Due to symmetry, the drag acting on these types of particles can be computed as either two- or three-dimensional problems.

The two-dimensional program was verified by studying spheres, cylinders and disks.[7] The two-dimensional analysis has been applied to single spherical particles, cylinders in cross flow, disk shape particles and spherical particles connected in chains. In all cases the shapes were selected because there was a prior determination of the drag force on the particle, either by analytical or experimental methods, and reported by other investigators, since it was the object of this portion of the project to gain confidence in a numerical technique. For the single spherical particle, the drag force from the numerical solution was compared to the drag force predicted by Stokes law. The results of this analysis for particle diameters of 2, 5 and 10 µm show that the calculation of the drag force on a particle agreed within 4% of that determined by Stokes law. For the case of cylinder in cross flow, which utilized rectangular coordinates, only one case was analyzed (10 µm diameter) and compared to the analytical solution. The difference was only approximately 2.5%. The disk in cross flow was studied utilizing cylindrical coordinates. The results of this test were compared to that of Oseen's solution. In the case of the disk, the analysis was run for several values of the Reynolds Number. The error in the drag forces increased with decreasing Reynolds Number from approximately 1 1/2% at a Reynolds Number of 0.13 to about 6% at a Reynolds Number of .00326.

Upon verification, the computational method was optimized and the technique expanded to include the three-dimensional case. For the three-dimensional case, test runs were performed on spherical and cubical particles. The numerically determined drag force on spheres was within 4.5% of the analytically determined value. For cubes, the values were within 5% of the experimental values reported in the literature.

Verification of Three-Dimensional Algorithms on Irregular Shaped Particles

The verification of the three-dimensional algorithm on regular shaped particles was encouraging. However, we felt that in the development of any numerical technique of this complexity, it is also important to compare the numerical results to experimental results, preferably obtained with a proven, standard method. For this reason a spiral duct centrifuge, which can provide information on the EAD of either regular or irregular shaped particles, was used to collect particles of several types. This instrument has been developed and used successfully for many years by investigators to determine the EAD of agglomerates of spheres and chain aerosols as well as irregular shaped particles.[8,9] In the centrifuge, particles are introduced into the center of a rotating spiral channel in which aerosol and clean sheath air are flowing. Particles introduced into the inner edge of the spiral channel are collected upon a foil attached to the outer edge of this channel. The distance from the introduction point to where the particles strike the foil is a function of their EAD, with the larger EAD particles being collected closest to the inlet.

The centrifuge used in this project was the Lovelace Aerosol Particle Separator (LAPS) which is used extensively by Lovelace Inhalation Toxicology Research Institute (ITRI). With the aid of ITRI personnel, several runs were made with coal, silica, and talc particles. This provided a variety of shapes for which the numerical technique could be applied. Sections from the centrifuge foils were removed at locations corresponding to aerodynamic diameters from 1 to 4 μm and the particles subjected to SEM analysis.

EXPERIMENTAL DETERMINATION OF PARTICLE SHAPE

The three-dimensional shape of an irregular shaped particle must be known in order to determine the EAD of the particle with the numerical computer program. However, inspection of the particles with the SEM only provides two-dimensional views of the particles. In our initial attempts to determine the three-dimensional shape of the particles, the shape and size of the particles in the third dimension were inferred from their two-dimensional shapes. This required that assumptions be made about the symmetry and regularity of the particles based on one two-dimensional view. It was realized that these assumptions could be erroneous. To eliminate the need for the assumptions in the third dimension, the particles were shadowed with a gold film in two orthogonal directions at an angle of 15° and then the particles and their shadows inspected with the SEM. The shadows were successful in providing views of the third dimension of the particles. This technique was very informative, in that the third dimensions of the particles were often drastically different than what we would have inferred from their two-dimensional shape. For example, a particle that looks like a sphere could in actually be a particle shaped like a disk or a spear.

Photomicrographs of four particles inspected in this manner are shown in Figure 1. These are three coal particles of various shapes and a talc particle. The particles in Figures 1a and 1b have projections protruding from the top of the particle. These projections would not have been suspected.

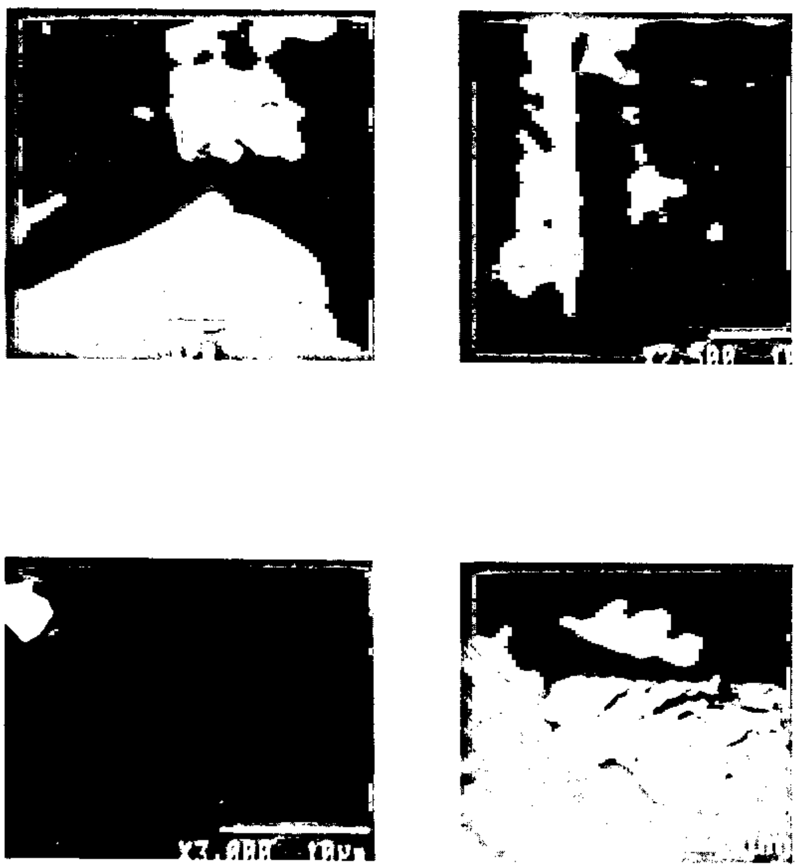


Figure 1. Photomicrographs of coal and talc particles shadowed in two orthogonal directions.

In some cases, the particles have multiple projections as shown in Figure 1c. The talc particle is a flakelike particle with a diameter approximately 10 times its thickness.

APPLICATION OF NUMERICAL TECHNIQUE TO CALCULATE AERODYNAMIC DIAMETER

The first step, in applying the numerical technique to determine the aerodynamic diameter of irregular shaped particles, such as shown in Figure 1, is to approximate the shape of the particles by a series of blocks as shown in Figure 2. The reason for approximating the particles as a series of blocks is that the numerical program is in rectangular coordinates and each cube in the three-dimensional array must represent either a portion of the particles or the space around the particles.

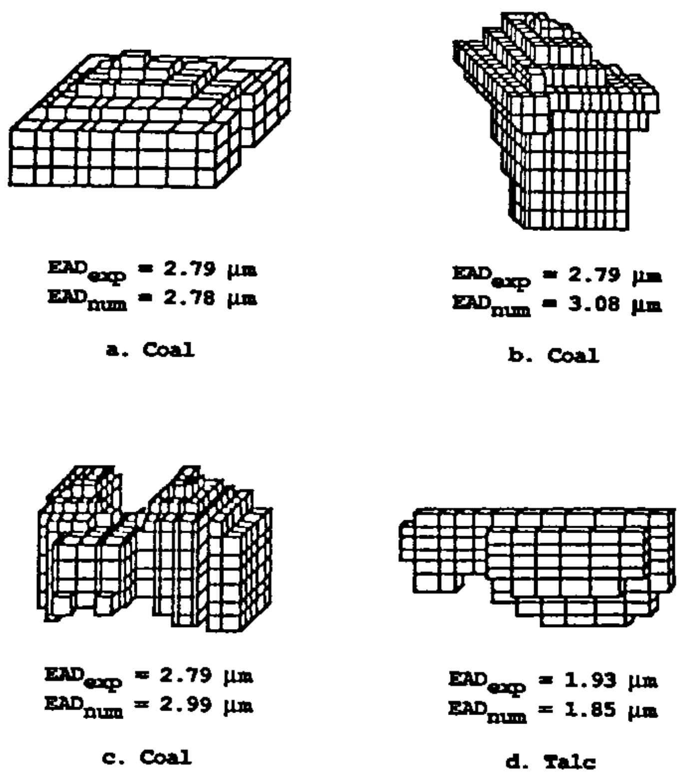
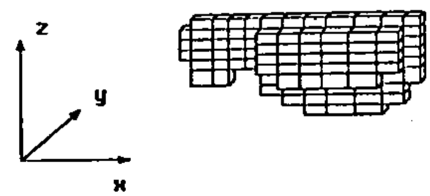


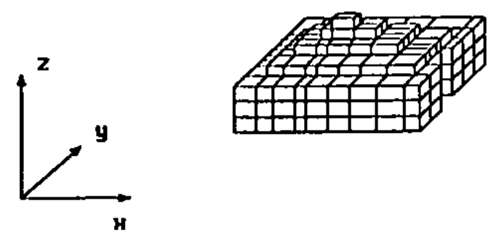
Figure 2. Digitized three-dimensional representations of particles in Figure 1 and a comparison of the numerically and experimentally determined EAD's.

Once the cubes within the three-dimensional array which represent a particle are identified, the viscosity in these cubes is set at a very high value. Therefore, when the flow field equations are solved over the entire domain (the domain of the particle plus the surrounding volume of approximately 10 times the particle diameter), the volume defined by the large viscosity will be considered as a solid within the domain and will not flow, while the volume around the particle will have the viscosity of air and will define the flow field around the particle. After the flow field has been determined, the drag on the particle can be calculated and, thus, its EAD determined. For each particle shown in Figure 2, the experimentally determined EAD from the centrifuge is compared to the numerical results. In most cases the agreement is quite good, especially since the orientation of the particle as it passes from the inlet to the foil in the centrifuge is not known. The aerodynamic diameter of the particle will be a function of its orientation as it moves toward the foil.

To determine the sensitivity of a particle's aerodynamic diameter to its orientation, the aerodynamic diameter in three orthogonal directions were determined numerically for two particles shown in Figure 3. The table associated with each particle indicate that the aerodynamic diameter is a function of its orientation. Note that the variation is only about 17% from their smallest to largest value of EAD's. Also, indicated



Direction of the flow	EAD,µm Numerical	EAD,µm Experimental
x	2.17	----
y*	1.85	1.93
z	2.10	----



Direction of the flow	EAD,µm Numerical	EAD,µm Experimental
x	2.89	----
y	2.92	----
z*	2.78	2.79

* Direction of the particle settling

Figure 3. Comparison of the numerically determined EAD's for three orthogonal orientations of a talc and coal particle.

in the table is the experimentally determined EAD corresponding to the direction that the particle was found on the foil. The agreement between these experimental values of the EAD's and the theoretical EAD's for the same orientation is very good.

CONCLUSIONS

A powerful tool has been developed for determining the EAD of an irregular shaped particle in any orientation. This technique utilizes the numerical solution of the Navier-Stokes equations in three dimensions and provides detail for the features of the flow around the particle, which leads to the calculations of the drag coefficient and EAD of the particle. The experimental verification of the theoretical technique has been quite satisfactory in that the aerodynamic diameter determined experimentally agreed with the theoretically determined values.

In the process of determining the three-dimensional shape of a particle in an SEM, it was found that the shadowing of the particle in two orthogonal directions was necessary. This shadowing revealed that inferring the three-dimensional shape of a particle from its two-dimensional projection is not satisfactory and that the shadowing is absolutely necessary if detailed information of the particle shape and size is to be obtained.

REFERENCES

1. Marple, V.A.: A Fundamental Study of Inertial Impaction. *Ph.D. Thesis* University of Minnesota (1970).
2. Rader, D.J., Marple, V.A.: Effect of UltraStokesian Drag and Particle Interception on Impaction Characteristics. *Aerosol Sci. Technol. 4:141-156 (1985).*
3. *Rader, D.J., Marple, V.A.: A Study of the Effects of Anisokinetic Sampling. Aerosol Sci. and Technol.* 8:283-299 (1988).
4. Patankar, S.V.: *Numerical Heat Transfer and Fluid Flow*. McGraw-Hill-Hemisphere Publication, New York (1979).
5. Gousman, A.D., Pun, W.M., Runchal, A.K., Spalding, D.B., Wolfshtein, M.: *Heat and Mass Transfer in Recirculating Flows*, Academic Press, New York (1969).
6. Marple, V.A., Rader, D.J.: Recent Developments in the Application of Finite Difference Solutions to the Study of Flow Fields and Particle Trajectories. Presented at the *Third Symposium on Advances in Particle Sampling and Measurement* held in Daytona Beach, Florida (October 18-21, 1982).
7. Marple, V.A., Zhiqun, Z., Liu, B.Y.H.: Numerical Technique for Calculating the Equivalent Aerodynamic Diameter of Particles. Presented at *International Symposium on Respirable Dust in the Mineral Industries*, University Park, Pennsylvania (October 14-16, 1986).
8. Stober, W., Flachsbart, H.: Size-Separating Precipitation of Aerosols in a Spinning Spiral Duct. *Environ. Sci. Technol.* 3:1280-1296 (1969).
9. Kotrappa, P., Light, M.E.: Design and Performance of the Lovelace Aerosol Particle Separator. *Rev. Sci. Instru.* 43:1106-1112 (1972).

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