FILTRATION THEORY USING COMPUTER SIMULATIONS*

by

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Abstract

We have used commercially available fluid dynamics codes based on Navier-Stokes theory and the Langevin particle equation of motion to compute the particle capture efficiency and pressure drop through selected two- and three-dimensional fiber arrays. The approach we used was to first compute the air velocity vector field throughout a defined region containing the fiber matrix. The particle capture in the fiber matrix is then computed by superimposing the Langevin particle equation of motion over the flow velocity field. Using the Langevin equation combines the particle Brownian motion, inertia and interception mechanisms in a single equation. In contrast, most previous investigations treat the different capture mechanisms separately. We have computed the particle capture efficiency and the pressure drop through one, 2-D and two, 3-D fiber matrix elements.

I. Introduction

Developing an accurate theoretical model of particle filtration is extremely difficult because of the complex nature of the filtration process, which involves particle transport in a fluid moving through a complex filter geometry. Figure 1 illustrates the complicated structure of a typical filter medium made from glass fibers. The fluid and suspended particles flowing through this fiber maze follow an extremely tortuous path controlled by the fluid dynamics and the particle equations of motion. Other type of filter structures such as spheres or granules and irregular porous structures are also frequently used in filtration.

The previous approach for modeling the particle filtration process has been to represent the complicated filter structure by a single element and then compute the fluid flow and particle transport around the one element.[1,2] The particle transport was computed by separately adding the contributions due to diffusion and inertia to the integrated trajectory. More recently, investigators have begun to model filtration in terms of parallel fibers arranged in a symmetric two-dimensional configuration.[3] Although this is an improvement over the single collector model, the filtration is still limited to 2-D flows through overly simplistic filter geometries.

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Figure 1. Scanning electron micrograph of glass fiber media used in high efficiency particulate air (HEPA) filters.

The problem with these previous approaches is that only general trends can be obtained from the computations, and considerable amount of experimental studies are still needed to substantiate the computations for specific filter designs and operating parameters. For that reason, filter designs and operational parameters generally are established through extensive experimental studies. This approach is both costly and time consuming. Perhaps even more important, the previous theoretical models restrict the development of new filters to existing production designs and available materials rather than what is theoretically possible. To overcome these deficiencies we have developed a filter simulation model that can simulate the filtration of suspended particles through more realistic filter structures, although not yet as complicated as that shown in Figure 1. The complexity of the fluid flow and particle trajectories through the filter media shown in Figure 1 greatly exceed present computer hardware and software capabilities, even when using advanced mainframe computers.

II. Development of Filtration Simulation Model

We have used commercially available fluid dynamics codes, NEKTON version 2.85, (Fluent Inc. 10 Cavendish Ct. Lebanon, NH 03766) and FIDAP version 6.0, (Fluid Dynamics International, Inc. Evanston, Il, 60201) and the particle equation of motion to compute the particle capture efficiency and pressure drop through selected two- and three-dimensional fiber arrays. The approach we used was to first compute the air velocity vector field throughout a defined region containing the fiber matrix. This was the most difficult and time consuming task in our study. Each combination of inlet air velocity and fiber matrix required a significant effort to set up the fluid problem and to compute the velocity field. All of the air flow calculations in this report were conducted with a uniform inlet velocity directed at the fiber matrix, and we allowed the exit velocity to vary. We did not force the fluid to be periodic (equal velocity fields at the inlet and exit) through the fiber matrix because of the additional work required to establish periodic flow.

The most difficult and time consuming step of the simulation is computing the velocity and pressure fields using computational fluid dynamics (CFD) computations. We have used the commercial CFD solvers, NEXTON and FIDAP, which are based on Navier-Stokes equations. The large memory requirements (5OMB) and the long processing times (20 hours) for the CFD computations limit the size of the filter model that can be studied to filter structures with about 100 fibers when using computer workstations. Using PCs would restrict the filter to about 10 fibers, while a supercomputer could compute structures with up to 1,000 fibers.

The filtration computer simulations require a UNIX based hardware platform with a minimum of 48MB of memory to run. We computed the filtration simulations that are shown in this report using the SGI Indigo platform from Silicon Graphics. The following are the software and hardware requirements:

Table 1. Hardware and Software Requirements For Computer Simulations

COMPONENT	REQUIREMENT
Graphics	Requires open/GL Graphics. 8 bit -planes is adequate
CFD Solver	A CFD solver is required. Any 3D CFD solver can be used, e.g. NEKTON or FIDAP. A mesh generator may also be required, e.g. TrueGrid.
Visualization	SGI's Explorer was used
Main Memory	48MB
Disk Storage	10MB minimum, primarily for flow fields

Figure 2 shows an example of the two-dimensional air flow calculations through a matrix of 2μm and 4μm diameter fibers. The inlet flow velocity was 20 cm/s. We were also able to compute the three-dimensional flow fields through the staggered hexagonal array in Figure 3 and the crossed fiber array in Figure 4. The direction of flow is in the X-direction. Once the air flow velocity field is determined, the differential pressure is also fixed and is read directly from the computer output.

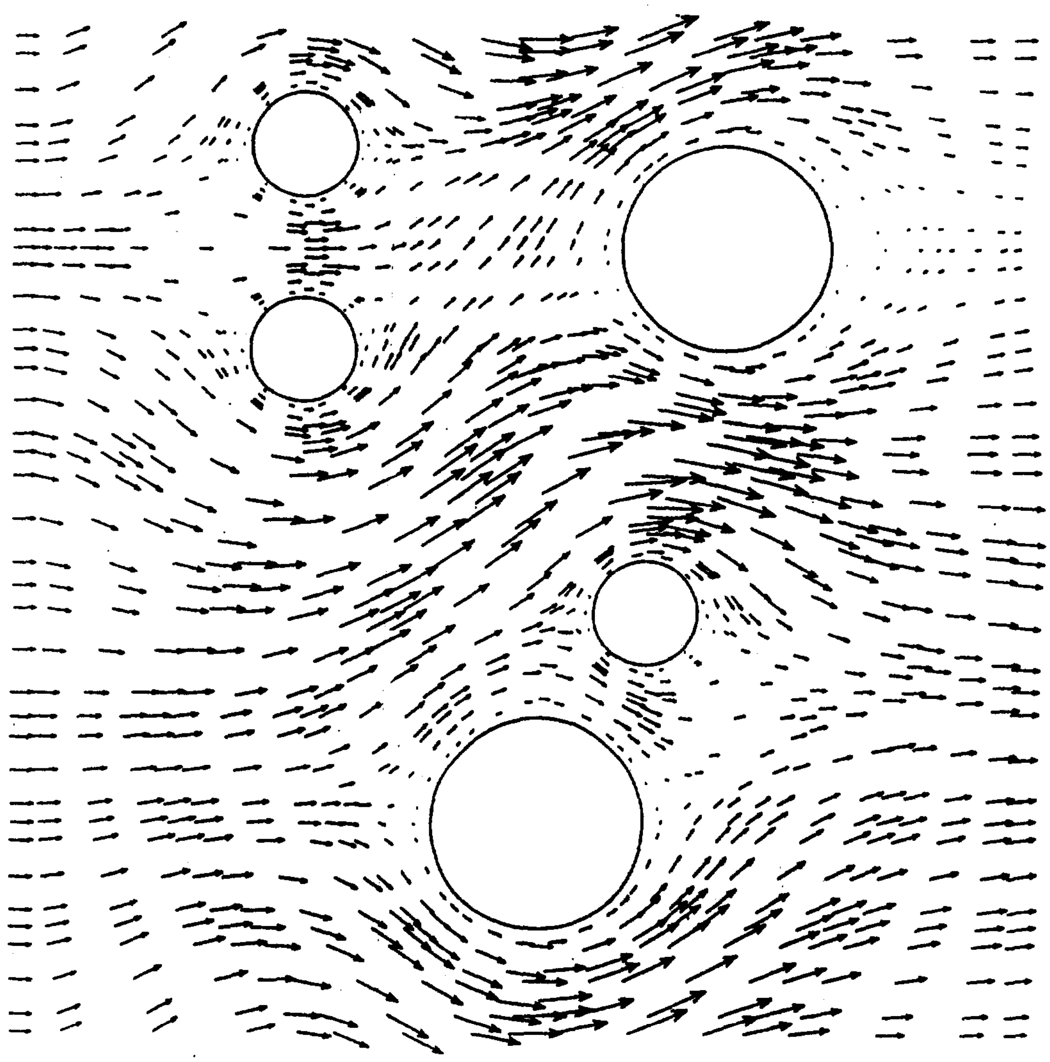


Figure 2 Air velocity vector field through 2-D fiber matrix at 20 cm/s initial velocity. The fiber matrix is 20μm x 20μm with 2 μm and 4μm diameter fibers. The fiber volume fraction is 0.0864.

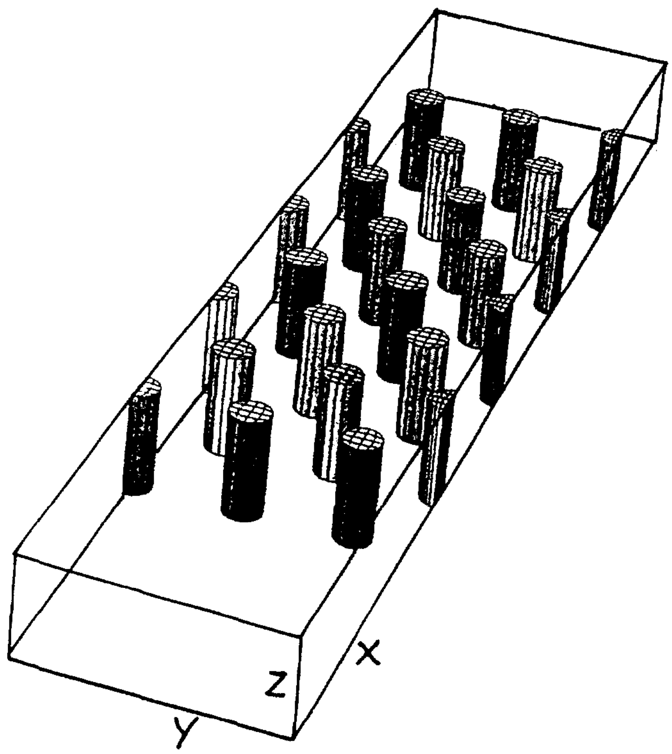


Figure 3 3-D fiber matrix with 1μm diameter fibers arranged in a staggered hexagonal array. The fiber matrix L x W x H is 23.0μm x 6.5μm x 5.0μm. The fiber volume fraction is 0.0825, and air flow is in X direction.

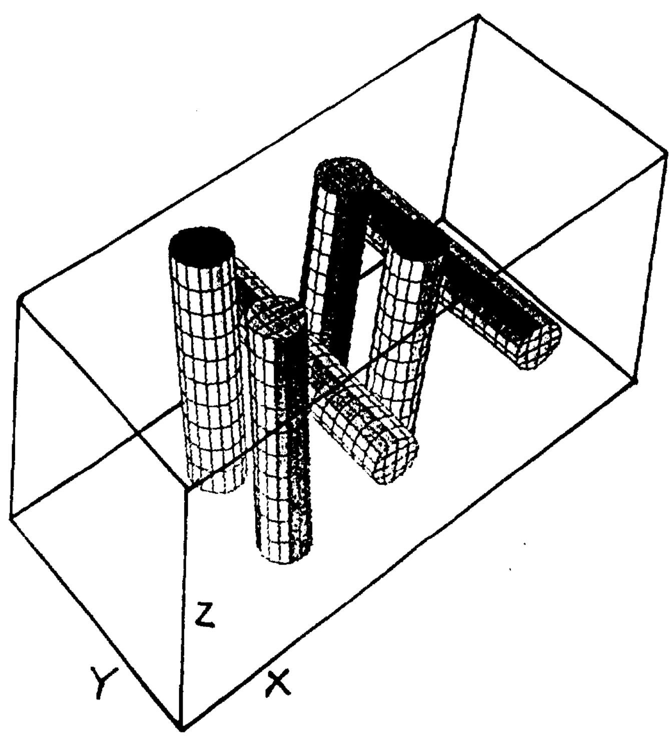


Figure 4 3-D fiber matrix with 1μm fibers arranged in a crossed fiber array. The fiber matrix L x W x H is 11μm x 5μm x 5μm. The fiber volume fraction is 0.0843 and air flow is in X direction.

The particle capture in the fiber matrix is then computed by superimposing the particle equation of motion over the flow velocity field. The resulting particle dynamics is given by:

$$\frac{d\underline{v}}{dt} = B(\underline{u}-\underline{v}) + \underline{A}(t) \qquad (1)$$

where,

- $\underline{v}$ = particle velocity vector
- $\underline{u}$ = fluid velocity vector
- B = friction coefficient
- $\underline{A}(t)$ = random Brownian acceleration, time dependent
- t = time

The friction coefficient B is defined as

$$B = \frac{6\pi\ \mu a_p}{C_s\ m} \qquad (2)$$

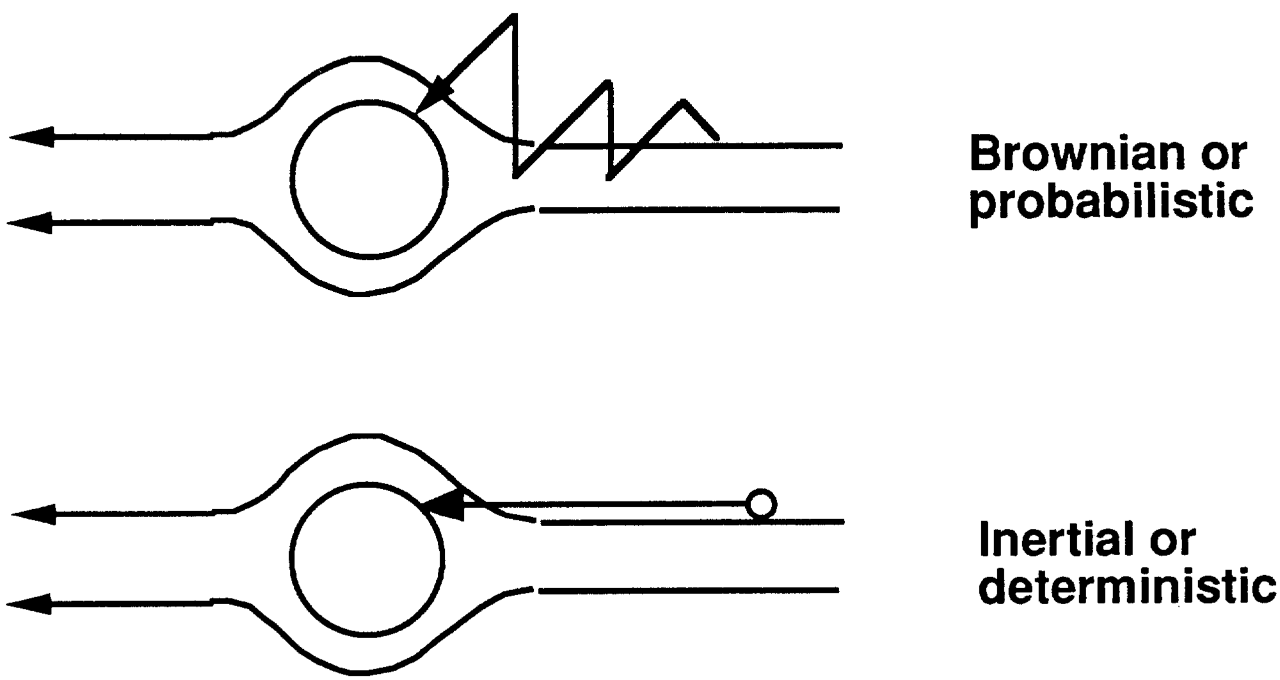
where,

- μ = fluid viscosity
- a_p = particle radius
- m = particle mass
- C_s = Cunningham slip correction factor

The solution of Equation 1, called the Langevin equation, can be obtained assuming a constant fluid velocity and a constant value of B.

Ramarao et al have solved Equation 1 using the method proposed by Chandrasekhar for two-dimensional particle trajectories.[4,5] We have extended this method to three dimensions in the present study. The principle of superimposing particle motion over the flow field is illustrated in Figure 5, where the net particle motion is the sum of a deterministic term and a probabilistic term.

Figure 6 shows the results of three, two-dimensional particle trajectories computed for the flow field in Figure 2 using Equation 1. Figure 7 shows the results of three, three-dimensional trajectories computed for the crossed fiber matrix. The inlet air velocity in both figures is 20 cm/s. The particle size in each of the three trajectory calculations was chosen to represent what is generally treated as three separate particle capture mechanisms: Brownian motion, interception and inertia. This artificial separation is not required for the general approach in Equation 1. Particle capture by the filter fiber only occurs if the particle trajectory contacts the fiber surface. Once particle contact is made, we assume the particle is captured and held tight. This assumption is valid for particles smaller than 5 µm at lower air flows.



$$\underbrace{\frac{d\vec{u}}{dt}}_{\text{particle motion}} = \underbrace{B(\vec{v}-\vec{u})}_{\text{deterministic}} + \underbrace{\vec{A}(t)}_{\text{probabilistic}} \qquad \text{Langevin eq.}$$

Figure 5. Particle motion is determined by the superposition of the Brownian (probabilistic) motion and the inertial (deterministic) motion over the flow field.

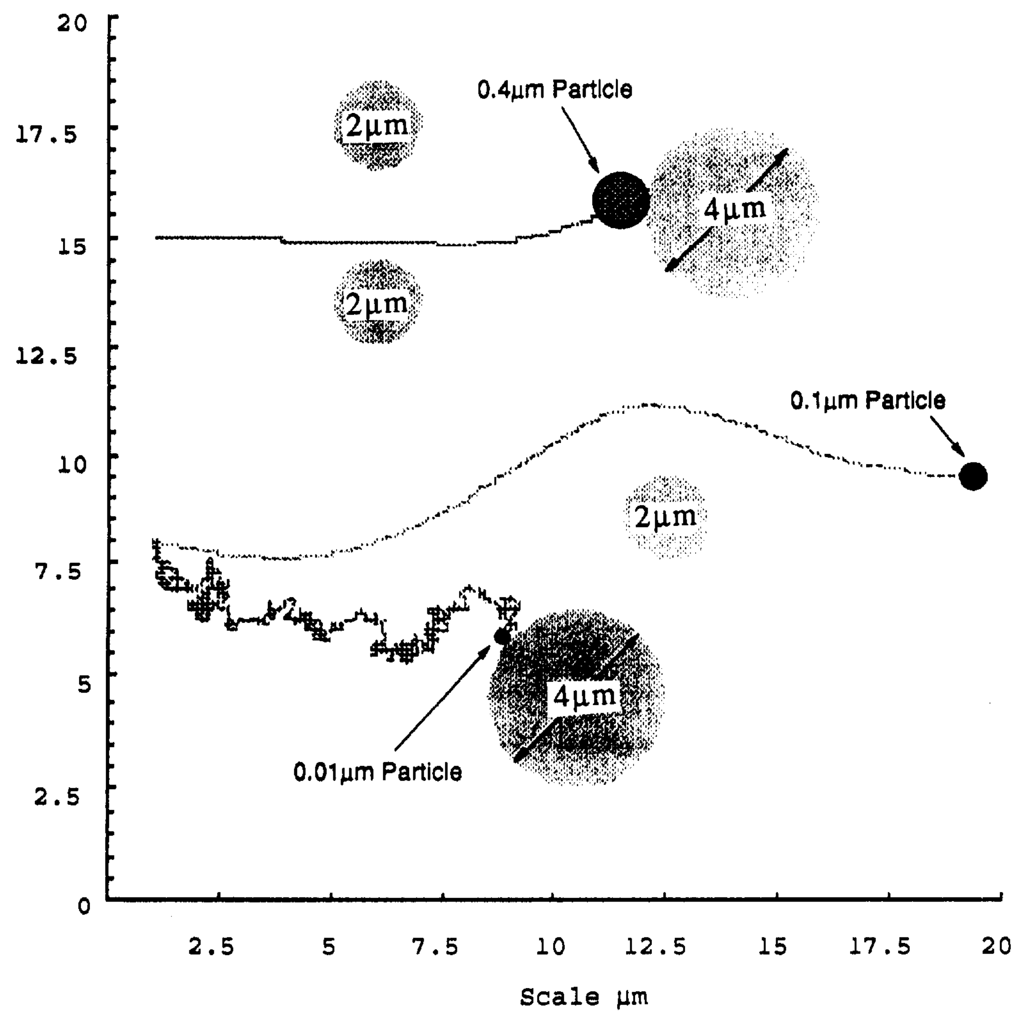


Figure 6 Trajectories of three different diameter particles through the fiber matrix in Figure 2. Particle diameters were selected to illustrate conventional mechanical collection mechanisms: 0.01μm for Brownian motion, 0.1μm for interception, and 0.4μm for inertia.

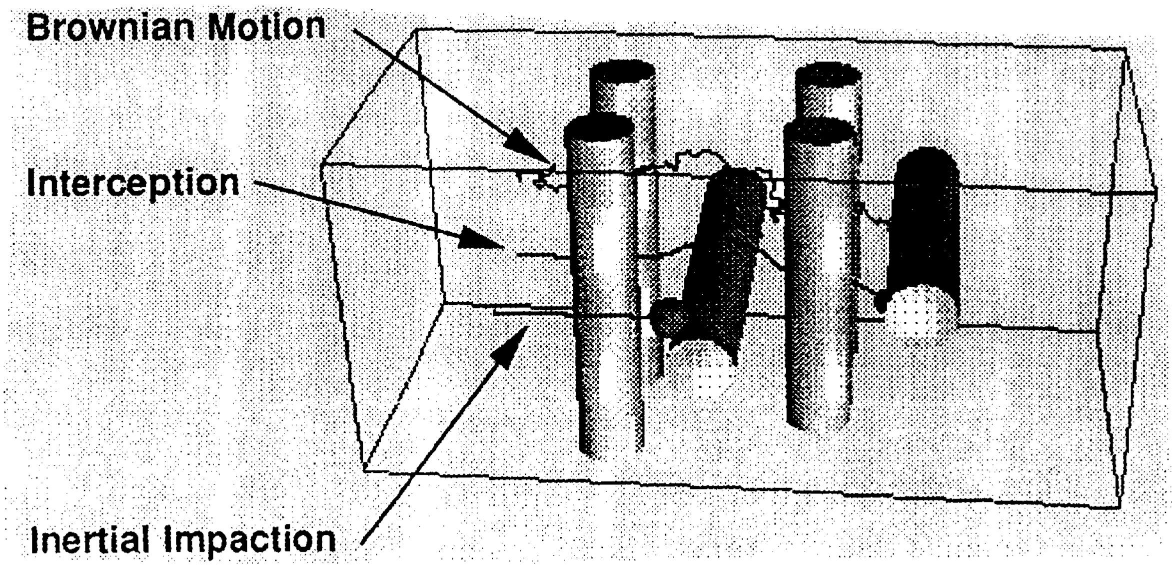


Figure 7 Trajectories of three different diameter particles through the fiber matrix shown in Figure 4 with the inlet air velocity at 20 cm/s. The diameter of the particles were selected to illustrate the conventional collection mechanisms due to Brownian motion, interception and inertial impaction. Note that the particle sizes are not to scale to allow visualization.

To determine the particle capture efficiency of a given fiber matrix for comparison with experimental measurements, it is necessary to compute thousands of trajectories for each particle size. For each trajectory calculation, the initial starting location is determined by a random number generation in the Y-Z plane. Figure 8 shows the cumulative efficiency of 0.3 μm diameter particles (density 1 g/cm^3) passing through the crossed fiber matrix as illustrated in Figure 7 with an inlet air velocity of 20 cm/s. Performing similar calculations at other particle sizes allows us to plot the efficiency versus particle size.

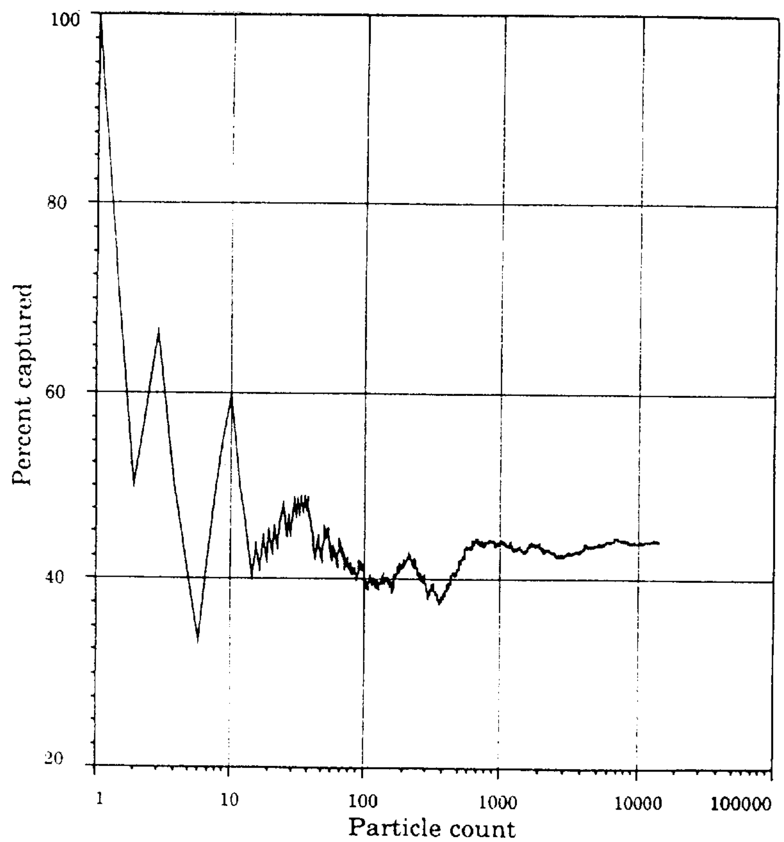


Figure 8 Cumulative efficiency of increasing number of 0.3μm diameter particles (density 1 g/cm^3) passing through the crossed fiber matrix in Figure 4 with a uniform inlet air velocity of 20 cm/s.

III. Sample Computations of Filter Efficiencies

The computation of the filter efficiency for a given fiber configuration and a given air flow requires three sequential steps: (1) compute the fluid flow field using CFD calculations, (2) compute the particle trajectory using Equation 1, and (3) compute the trajectories of many particles at random positions at the filter inlet to obtain an average efficiency. These calculations will yield the efficiency at a given particle size. For filter efficiency as a function of particle size, steps 2 and 3 must be repeated for each particle size. For efficiency at different air flows, all three steps must be computed.

Figure 9 shows the results of the efficiency calculations for the crossed fiber array at 20 cm/s. Figure 10 shows the efficiency of the same crossed fiber array at 2 cm/s. Note that the capture efficiency for the larger particles increases while the efficiency for the smaller particles decreases as the air velocity is increased. Figure 11 shows the particle capture efficiency for the staggered hexagonal array at 3 cm/s.

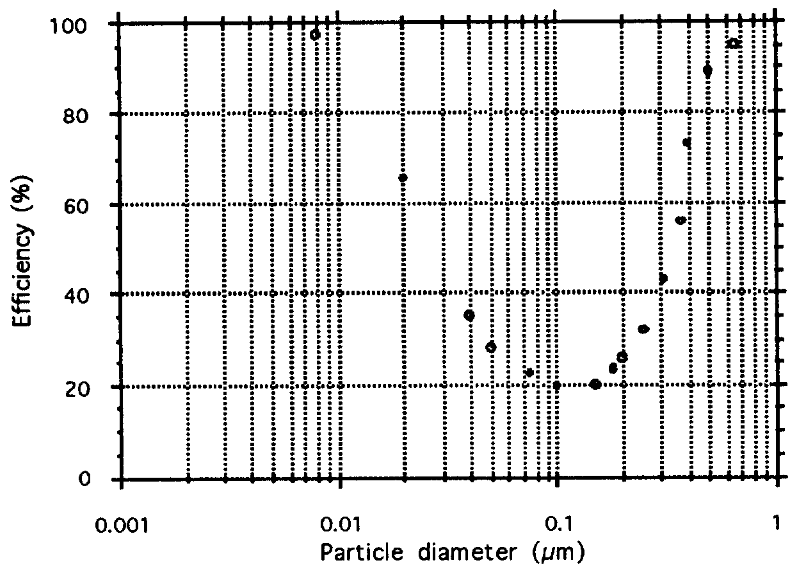


Figure 9 Filter efficiency computed for different particle diameters (density 1 g/cm^3) passing through the crossed fiber matrix in Figure 4 with uniform inlet air velocity of 20 cm/s. The pressure drop across the fiber matrix element is 4.4 x 10^{-5} inches of water.

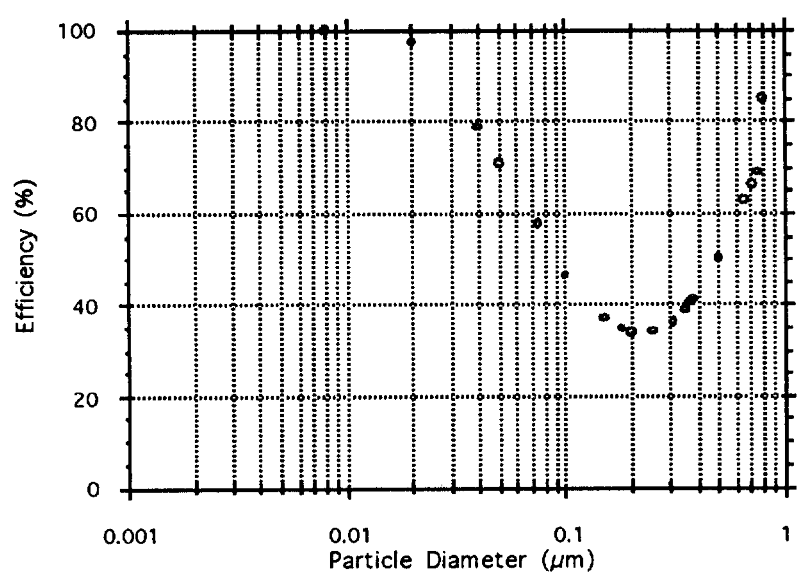


Figure 10 Filter efficiency computed for different particle diameters (density 1 g/cm^3) through the crossed fiber matrix in Figure 4 with a uniform inlet air velocity of 20 cm/s. The pressure drop across the fiber matrix element is 4.4 x 10^{-6} inches of water.

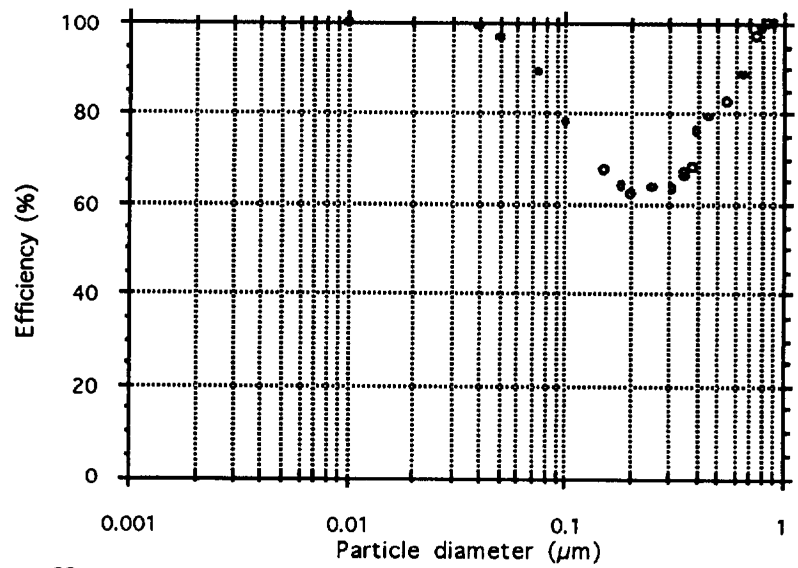


Figure 11 Filter efficiency computed for different particle diameters (density 1 g/cm^3) through the staggered hexagonal array in Figure 3 with a uniform inlet air velocity of 3 cm/s. The pressure drop across the fiber matrix element is 3.2×10^{-5} inches of water.

Although it is feasible to compute the particle capture efficiency and pressure drop across simple fiber matrices as shown in this report, we are a long way from computing the efficiency and pressure drop for commercially available filters. The primary limitation here is an efficient method for computing the fluid flow through the more complicated fiber matrix in real filters.

IV. References

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4. Ramarao, BV, Tien, C, and Mohan, S "Calculation of single fiber efficiencies for interception and impaction with superimposed Brownian motion" J. Aerosol Sci., Vol 25, No. 2, pp 295-313, (1994).

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DISCUSSION

WEBER: I think that the work that Werner is doing is a real service to the industry and I hope that he will be able to carry out his plan to bring it to full fruition. I have a couple of questions for the author. Do you have a way of measuring the fiber diameters in a large assembly?

BERGMAN: We determine fiber diameters from electron micrographs followed by computer scanning and generate histograms of the number of fibers versus size. For three dimensional analysis, we solidity the filter element with an epoxy, take slices of the element at increasing depths and then take SEM photos. For quicker, less expensive analysis, we simply took SEM pictures of the media surface.

WEBER: I noticed that the fiber diameters you cited were greater than $1\mu m$ yet we know that the glass fibers optimally used are less than that in many cases. Was there a particular reason for the choice of diameter in your calculations?

BERGMAN: Yes. Below $1\mu m$ you have non-continuum fluid dynamics that is often called "slip" flow. All of the conventional fluid dynamics codes are based on a continuum fluids. To address the slip flow, we first compute the flow using continuum mechanics and then close to the fiber, we introduce an empirical term. This approach is not rigorously correct, but it yields better results than ignoring slip. Using a noncontinuous fluid dynamics package in filtration modeling would greatly exceed the capacity of the largest computer.

WEBER: Finally, I am wondering how long through the useful life of a filter it would be until cake build-up or the presence of previously deposited particles would affect the result, or would start to dominate the result?

BERGMAN: We did not do these computations. From the pictures of particle trajectories, you can see that it is possible to model filter clogging. Let me illustrate how this can be done. For the initial particle capture and deposits, we assume the general fluid dynamics flow is not affected by the deposits. However, once the deposits become sizable, you have to recompute the fluid field with the altered filter geometry. Particle trajectories are then computed for the new fluid velocity field and a new increment of deposits formed. The cycle of forming particle deposits and computing new flow fields is repeated many times. Considering that it may take 20-40 hours of computer processing on a silicon graphics workstation to compute the flow field in a 100 fiber filter element, we are a long way from realistic filter clogging simulations.

KOVACH, B: The work you did is great but did you consider the influence of a vibrating fiber due to high velocity airflow? Would it increase or decrease the efficiency? Is your video movie available for use by others?

BERGMAN: As soon the work is finished we will make copies available. With regard to vibrating fibers, I am not aware of any studies. However, if you look at the period of vibration, I suspect the period would be much longer than the effective residence time of a particle in the vicinity of a fiber. I have a difficult time imagining a fiber vibrating at a speed that is comparable to the particle velocity, but then I've been surprised more times than not.

THOMAS: Previously, I tried to use equations by Drs. Liu and Rubo to determine filter efficiency, but I ran into a problem trying to determine their parameter for collector diameter. I used an average fiber diameter, but I was wondering if you have determined any kind of average filter fiber diameter based on information from people that make filter papers?

BERGMAN: Although we can determine fiber size distribution precisely, the problem is that the paper is very heterogeneous. The fiber diameter distribution and fiber volume fraction can vary greatly depending on where the measurments are taken in the filter paper. The common practice is to use an "inhomogeneity factor" and an average fiber diameter derived from SEM pictures in a specific filter equation for pressure drop. The inhomogeneity factor is used to force agreement between the equation and experiment. Since all of the pressure drop theories (Karmen-Kozenly, Kuwabara, etc.) have pressure drop varying inversely proportional to fiber diameter squared, the most common average is the weighted average of diameter squared. The weighting factor generally is a function of the site distribution and the distribution of fiber volume fraction throughout the filter. A more practical approach is to use an "effective" diameter which is the diameter determined from the pressure drop equation with experimental pressure drop data.

DYMENT: Does the speaker consider an attempt should be made to include electrostatic forces? Can the techniques described be used to produce designs of filter media having extended dust capacity?

BERGMAN: We have added electrostatic forces in the computer models but have not run many cases. I should add that any number of additional capture mechanisms can be easily added to the code because once you have established the flow field and the mechanical trajectory, it is a minor step to add additional capture mechanisms. The current stage of computer simulation can be used to investigate extended life, but it is not practical because of the excessive time required to compute. The problem is that each time the morphology of the particle deposits changes it perturbs the air flow and therefore requires a new flow field computation. An entire series of flow computations would be required for each filter media structure. This would require an enormous amount of computation and is not practical at the present time.

DYMENT: I have been fascinated by your demonstration, I think it is a major step forward. Filtration is an extremely complex process. Do you imagine we use the filters that electrical effects are significant because you are studying what we call mechanical effects. Do you think that electrical effects can be important in real filters? That is my first question. My second question concerns the graded papers we were talking about at the last conference which have a somewhat higher dust holding capacity. Do you anticipate that you can use these techniques to give us target designs for filters which will hold larger quantities of particles before their resistance rises to the point at which we have to change them?

BERGMAN: If conditions are favorable for electrical effects, then they will be very important in filtration. Conditions that favor electrical effects are dry air, charged particles, and high filter electrical resistance. Thus I would expect electrical effects would enhance the performance of real filters in dry air powder handling or processing operations. Applications involving aqueous oil mists or ambient aerosols would have little electrical effects. The computer simulations can be used to answer performance and design questions, but only for very simple systems at the present time. Even the simple filtration problems illustrated in this paper require 3-4 days of work. Setting up the basic filter structure represents currently about 10% of the effort. Fluid dynamics represents 80% of the full effort. The particle trajectories represent 9% and the remaining 1% is the electrostatics. The purpose of this presentation is to begin the process of developing a CAD/CAM system where engineers can sit at their computers and calculate the filter efficiency for graded efficiency filters, unusual structures, filter clogging, whatever it is you want. Major advances in both computer software and hardware will be required this goal.