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Aerosol Filtration by Fibrous Filters: A Statistical Mechanics Approach

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Abstract A statistical mechanics approach, namely the Ising model combined with Monte Carlo simulation, was employed in studying the process of aerosol filtration through fibrous filters. This process was modeled as consisting of numerous cells' state exchanges driven by the difference of the system energy after and before a particle moved from one cell to the other and/or deposited on a fiber cell. With the use of a simpler binary algorithm, this approach was capable of realistically simulating the complicated mechanisms involved in the filtration process. Simulations were carried out for the behaviors of aerosol particles of different sizes interacting with isotropic fiber filters of various volume fractions. Simulation results were in good agreement with reported experimental data, indicating an encouraging prospect for the method to be applied in this area.

Key words aerosol filtration, fibrous filters, Ising model, Monte Carlo simulation

One of the most common methods of separating and removing particles in micro and sub-micro size range, aerosol filtration by fibrous filters, has found diverse applications, such as in the protection of humans and delicate devices from exposure to hazardous fine particles. It has, therefore, been the subject of active research, both theoretical and experimental.

The ability of fibrous filters to collect aerosol particles is usually expressed in terms of filtration efficiency, the fraction of entering particles that are retained by the filter. The efficiency of fibrous filters in collecting aerosols is often derived from the aerosol filtration efficiency of a single filter element (η), whose size and shape are chosen to best represent the microstructure and porosity of a given filtering material [1, 2]. The single fiber efficiency is the combined effects of the various mechanisms of capture, including direct interception, inertial impaction, diffusion deposition, gravitational settling, etc. [1, 2]. These mechanisms are not necessarily independent. Adhesive forces involved in filtration process are also studied. These forces include van der Waals forces [2, 3] and electrostatic forces [4, 5] between particle and fibrous filters.

However, the arrangement formats of fibers in a filter will always have great impact on the aerosol filtration since fibers interact during filtration process. The most difficult thing in studying aerosol filtration processes is the description of the heterogeneous fibrous structures. To account for the effect of fiber arrangement, two multifiber models have been used to investigate the interception efficiency of fibrous filters composed of symmetrical arrays of fibers, including parallel arrays and staggered arrays [6, 7], in which the filtration process was simplified as a two-dimensional periodic flow. Shapiro [8] introduced an inclusion model, where the filter material was regarded as a uniform

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matrix containing a certain volumetric fraction of inclusion of a certain size. Both inside and outside the inclusion, the filter structure was assumed to be homogeneous, albeit with different porosities. Alternative approaches [9] have involved a model where filter media were represented by a two-dimensional distribution [10] of cells of varying packing density.

When the filter structure is defined, the flow field during filtration can be characterized by such constitutive equations as continuity equation and Darcy's law. The constitutive equations and corresponding boundary conditions can be solved analytically or numerically to give the pressure field and velocity field. These relations, combined with expressions for single fiber efficiency, allow calculation of the efficiency of each element of the filter (local efficiency), as well as their combination or averaging into the overall efficiency of filter materials [9, 11].

However, any of these reported models is still not as precise as required for describing the heterogeneous structure of a fibrous filter and the stochastic nature of aerosol behavior. Other discrete approaches have, therefore, been attempted to deal with the problem involving heterogeneous structures. These approaches include lattice Boltzmann (LB) model [12] and Cellular Automata (CA) probabilistic model [13]. The CA models keep track of the many-body correlations and provide a description of the fluctuations, while the LB models are believed to be numerically more efficient and offer much more flexibility to adjust the fluid parameters [13].

In this paper, a statistical mechanics model, the Ising model combined with Monte Carlo simulation, is introduced as a new approach to the study of aerosol filtration by fibrous filters. The Ising model was first presented to study the phenomenon of ferromagnetic phase transition [14]. Since then it has been frequently used to study a system consisting of interactive subsystems, each of which bearing two interchangeable states [15–18]. In the Ising model, a real system is divided by a grid into discrete systems composed of a number of lattice cells. The filtration system was treated in this work as a system made from such subsystems as fiber cells and aerosol particle cells that interacted with each other through adhesion. The transport and deposition process of the particles in the fibrous substrate was due to interactions as well as the effect of moving air stream, resulting in each particle moving from one cell to the other. In general, such a change in the system's configuration is driven by the energy difference after and before the change, subject to the random fluctuations represented by Monte Carlo simulation. Allowing use of a simpler binary algorithm, the Ising model made for much greater accuracy and efficiency in simulation.

Model Description

The Ising Model

To describe the filtration process through a fibrous filter, a discrete three-dimensional Ising model is proposed. The system is divided into a lattice of a number of cubic cells. The length of a single cubic cell can be chosen arbitrarily and, for the sake of convenience, is made to be equal to the diameter of a fiber in this work.

To represent the possible states of each cell, two variables are introduced:

i) s_i, indicating whether a cell i is occupied by a particle ($s_i = 1$) or not ($s_i = 0$);
ii) F_i, showing whether a cell i is filled with fibrous substrate ($F_i = 1$) or not ($F_i = 0$).

Energy of the system (the Hamiltonian) should be the summation of the energies of each single cell H_i, which in turn is the summation of the interactions between the cell i and its 26 nearest neighboring cubic cells (see Figure 1), as

$$H_i = A\sum_j s_i s_j - \left(Bs_iF_i + C\sum_j s_iF_j\right) + Gy_i \tag{1}$$

This equation takes into account all three types of interactions:

i) Cohesive interaction between neighboring particle cells, as shown in the first term on the right hand side of the equation, A representing the cohesion energy between particles, and the summation of s value is over all nearest neighboring cells of cell i;
ii) Adhesive interaction between particle and fiber substrate, shown as the terms in the bracket, where B and C correspond to the adhesion energies between a particle and a fiber substrate in the same cell, and that in the nearest neighboring cells, respectively;

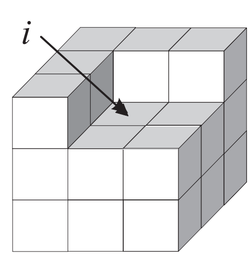

Figure 1 A cell *i* in a three-dimensional Ising model with its neighbors.

iii) Gravitational effect of particles as shown in the last term, where G is the intensity of the gravity field and y_i the y-coordinate of cell i in the lattice.

The coefficients in equation (1) are determined in a manner described as follows:

We assume that the van der Waals forces dominate the interactions between fiber and particles. According to the Lifshitz theory [19], the interaction energy between a particle (sphere) of diameter d_p and a surface, and that between two particles (spheres) with diameters d_{p1} and d_{p2}, can be expressed as equations (2) and (3), respectively:

$$W_{1,2} = -(h_{1,2}d_p)/12D \quad (2)$$

$$W_{1,2} = -\frac{h_{1,2}}{12D}\frac{d_{p1}d_{p2}}{(d_{p1}+d_{p2})} \quad (3)$$

where $h_{1,2}$ is the Hamaker constant and D the distance between the particle(s)/surface. An approximate expression for the Hamaker constant of two bodies (1 and 2) interacting across a medium 3, none of them being a conductor, is

$$h_{1,2} = \frac{3hv_e\left(n_1^2 - n_3^2\right)\left(n_2^2 - n_3^2\right)}{8\sqrt{2}\left(n_1^2 + n_3^2\right)^{1/2}\left(n_2^2 + n_3^2\right)^{1/2}\left\{\left(n_1^2 + n_3^2\right)^{1/2} + \left(n_2^2 + n_3^2\right)^{1/2}\right\}} + \frac{3}{4}k_B T\frac{\varepsilon_1 - \varepsilon_3}{\varepsilon_1 + \varepsilon_3}\cdot\frac{\varepsilon_2 - \varepsilon_3}{\varepsilon_2 + \varepsilon_3} \quad (4)$$

where h is the Planck's constant, v_e is the main electronic adsorption frequency in the UV (assumed to be the same for the three bodies and typically around 3×10^{15} s^{-1}), n_i the refractive index of phase i, ε_i the static dielectric constant of phase i, k the Boltzmann constant and T the absolute temperature.

Two constants k_1 and k_2 are used to represent the ratios of A/C and B/C, respectively.

$$k_1 = \frac{A}{C} = \frac{W_{1,1}}{W_{1,2}} = \frac{h_{1,1}}{h_{1,2}},\quad k_2 = \frac{B}{C} = \frac{h_{1,2}/2D_2}{h_{1,2}/D_1} = \frac{D_1}{2D_2} \quad (5)$$

The ratio A/C is equal to the ratio of the cohesive energy between two particles to adhesive energy between a particle and fiber in neighboring cells. As the interaction distances in two cases are the same, the ratio is also equal to the ratio of the Hamaker constants in the two cases. B/C is the ratio of particle/fiber adhesive energy in the same cell to that in the neighboring cells and, therefore, equals the ratio of the interaction distances. For interactions between a pair of neighboring particle and fiber cells, the distance, D_1, is assumed to be one half of the cell length, while for interactions of particle/fiber within a cell, the distance, D_2, depends on the scale of the surface roughness. In the present work, the value of C is determined by simulation to accommodate the experimental data and the values of A and B are determined by equation (5).

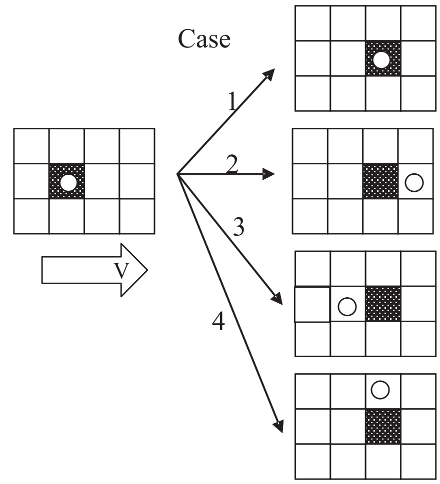

Figure 2 Energy difference due to airflow.

The transportation process of aerosol particles through the fibrous substrate is usually accomplished by airflow in a certain velocity. The usual thermodynamic theories specify the considered bodies/systems in a state of absolute equilibrium, whereas aerosol particles transport through fibrous structures in airflow is conventionally categorized in aerodynamics, and it comes with substantial friction loss of transport characteristic of irreversibility. Therefore, dealing with such a problem we have, on the one hand, to make statistical calculations and, on the other, compelled to take into mechanical energy terms like work of drag force. Assuming a quasi-equilibrium process this way, it is appropriate to extend Monte Carlo simulation [16] to the case of aerosol particles transport through fibrous filters in an airflow:

When a particle is suspended in airflow of velocity V, through one time step in which air moving from its original cell to a neighboring cell, the particle can move in four different ways (Figure 2), subject to different probabilities:

i) In the first case, the particle moves with the air stream to the neighboring cell. Accordingly, there is no relative velocity between particle and air stream during this time step and the work done on the particle by airflow can be regarded as zero;
ii) In the second case, the particle moves to a cell ahead of that of the air, with a velocity V relative to the air. The system energy change (dE) in this time step

includes both the change in Hamiltonian, dH, and the work done to the particle by airflow, W_A, as:

$$dE = dH + W_A = dH + F_D l \quad (6)$$

where l is the size of a cell, F_D is the drag force act on the particle with diameter d by the air stream and can be calculated according to the Stokes' Law as

$$F_D = 3\pi\eta\, dV \quad (7)$$

where η is the viscosity of air which, at standard pressure and room temperature, is 1.81×10^{-5} Pa · s;

iii) In case three, the particle remains in the original cell despite of the moving of air, the relative velocity of the particle to the air is –V. Therefore, the system energy change should be

$$\begin{aligned} dE &= dH + F_D(-l) = dH + 3\pi\eta d(-l)(-V) \\ &= dH + 2\pi\eta dlV \end{aligned} \quad (8)$$

iv) In case four, the particle may deviate from the air stream and move to other neighboring cells, as is the result of the combination of either the above three mechanisms or the diffusion. The influence of diffusion can be represented by the random effect of the Monte Carlo simulation described in the next section.

The energy difference in each case is then used in the Monte Carlo simulation to provide the probability for a cell to change its state at each time step.

Monte Carlo Simulation

In all the simulations in the present study, for the sake of simplicity, movement of fibers is neglected. That is, the filtration process is assumed not to alter the internal structure of the fibrous filter, so that values of F for all the cells are kept constant in a simulation. Therefore, the process of aerosol filtration is the result of each particle moving from one cell to the other and/or depositing on the fiber substrate in a fiber cell. Procedures of the simulation are as follows:

i) Initial configuration is created by developing the lattice, within which the fibrous media are laid. The initial values of both F (1 or 0) and s (1 or 0) for each cell are also determined. A cell i is considered to be covered with fiber (F = 1) if the distance between the cell center and the fiber axis is smaller than the fiber radius;

ii) All the particles in the space are scanned. For example, a particle cell i in the lattice is randomly selected. It can move in four different ways as described in the last section (also in Figure 2). For each case, dE (energy difference between the configurations before and after the change) is calculated. Then the case with the lowest value of dE is selected as the most probable change. If a random number uniformly distributed between 0 and 1 is chosen and is smaller than the spin-flip probability, $p = \exp(-\beta\Delta E_T)$, the change of configuration takes place. Here, β is a constant inversely proportional to the absolute temperature;

iii) A Monte Carlo step ends when all the particles in the current state have been scanned. Then step ii) is repeated to start a new Monte Carlo step until the whole simulation is terminated.

In the present study, a Monte Carlo (MC) step is defined as the time in which air moves from one cell to a neighboring one with size l. Therefore, if the velocity of air is V, the relationship between a MC step and real time is

$$1 \text{ MC step} = \frac{l}{V} \text{ (sec)} \quad (9)$$

Results and Discussion

Based on the above description, a computational simulation algorithm was developed for the process of aerosol particles of different sizes filtering through isotropic fibrous filters with different fiber volume fractions.

Experimental data were adopted from literature [20]; the filter used for testing was made from a polyester fiber, Dacron, of 12.9 μm in diameter. The filter fiber volume fraction was 27.1%. The particles were mono-disperse aerosols generated from dioctyle phthalate (DOP) solutions of different concentration to give different aerosol particle sizes.

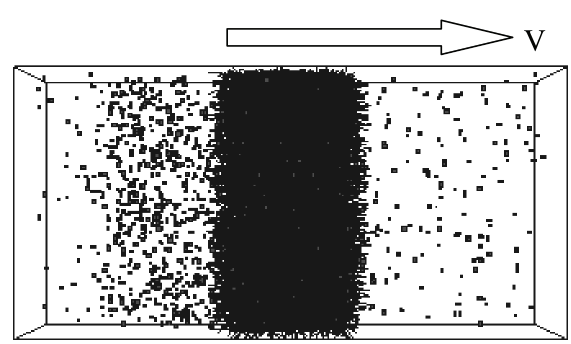

Figure 3 A three-dimensional Ising model for the filtration process.

Table 1 Parameters for fiber and aerosol particle at room temperature (20 °C) [21].

	Density ρ (g/cm^3)	Refractive index n	Static dielectric constant ε	Simulation parameters			
				A	B	C	β
Fiber (Dacron)	1.350	3.0	1.610	2.23×10^{-3}	15	1.86×10^{-3}	40
Aerosol particle (DOP)	0.983	5.1	1.485				

To start the simulation, the length of a cubic cell was made to be equal to the fiber diameter, 12.9 µm. The fiber mat was constructed by generating a certain number of fibers whose center points and orientations were randomly determined. Next, the fiber volume fraction was represented by the ratio of the number of cells that were occupied by fibers to the total number of cells. The simulated system comprised a lattice of $228 \times 100 \times 50$, as shown in Figure 3. The boundaries were periodical. In the space to the left of the fibrous filter, where the in-streams of the aerosols came from, the particles were regenerated after each Monte Carlo step to maintain a constant input aerosol concentration C_{in} (the ratio of the number of particles to the total lattice cells on left sides of the filter). When output aerosol concentration C_{out} (the ratio of the number of particles to the total lattice cells on right sides of the filter) reached equilibrium after certain Monte Carlo steps, filtration efficiency of a fibrous filter was calculated as the ratio of C_{out} to C_{in}:

$$E_F = 1 - \frac{C_{out}}{C_{in}} \qquad (10)$$

It has been suggested that the adhesive force on a particle less than 10 µm is much greater than other forces that a particle experiences [2]. The sizes of the particles modeled in this work were well below 10 µm. Gravity effect in equation (1) was, therefore, neglected.

The parameters needed for the simulation are listed in Table 1. This model applies to different fibers and particles by taking account of the property parameters for different materials. It can also be seen that interactions between neighboring cells (A and C) were in a much smaller scale than that within the same cell (B). This gap would be reduced in a finer lattice in cases of fibrous filters with more intricate structures e.g. nano-fiber filters.

Both simulation results (shown as continuous lines) and reported experimental data [20] (shown as discrete symbols) are shown in Figure 4. They were in high accordance, indicating a good validity of the method.

Both the simulations and experiments showed that, with the variation of particle size, the filtration behavior went first through a diffusion regime, where filtration efficiency decreased with increasing particle size, as smaller particle size made for better diffusion and thus better filtration efficiency. Then there was a regime of diffusion transiting to interception, and the efficiency went down to a minimum, where the dominance of diffusion mechanism was taken over by interception, and then rose with the increase of particle size. Finally in an interception regime, filtration efficiency rose singularly with particle size. Combination of the above mechanisms in the simulation process is represented in the energy expression in equations (6–8). To be specific, when the gravity effect can be neglected (for particle size below 10 µm):

i) Increased particle diameter d means higher adhesion between particle and fiber and the particles have fewer chances to deviate from the airflow. This leads to a more prominent impaction/interception mechanism;
ii) With decreasing particle diameter, on the one hand, adhesion between particle and fiber is weakened, and it becomes easier to remove a deposited particle from the fiber. On the other hand, the effect of airflow on the particles diminishes, and the particles have more chances to fluctuate around the streamline. Both of these factors contribute to enhanced diffusion.

Hence, the advantages of the present approach are first, the Ising model was capable of describing such complicated sys-

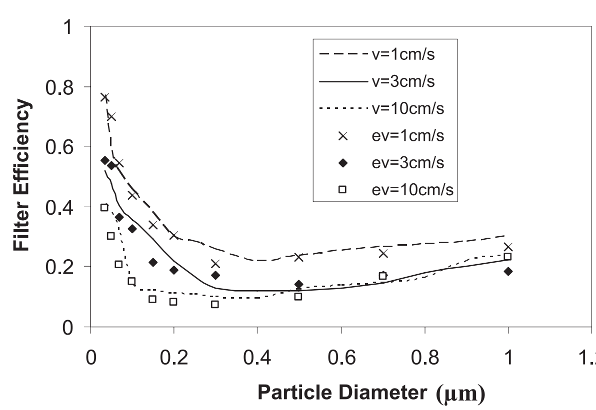

Figure 4 Simulation and experimental results of filter efficiency versus particle size.

tems as aerosol filtration in fibrous structures in a simple binary form, accounting for all the physical mechanisms involved, without using such indirect parameters as single fiber efficiency, as is the case with classical filtration approaches, yet generated robotically informative results. Second, the approach was obviously able to depict the intricate interface between aerosol and fibrous media. This approach could be especially useful for explaining effect of the interactions that occur at the interface within heterogeneous materials. Further, this model could be adapted to deal with more complicated cases, such as poly-disperse particles filtration through multi-layer fibrous filters.

However, since this work was intended to deal with a particle/fiber system where movement of fibers was neglected for the sake of simplicity, the model requires to be further modified if it is to be applied to study aerosol-fiber systems with considerable fiber movement, in which the parameter F for each cell has to change accordingly to reflect the fiber movement.

Conclusions

The study applied a statistical mechanics approach (i.e. the Ising model combined with the Monte Carlo method) to the aerosol filtration process through fibrous filters. The filtration system was treated as made from such subsystems as fiber cells and particle cells that interacted with each other through adhesion. The transport and deposition process of particles in the fibrous substrate was due to interactions and the effect of the moving air stream as well, resulting in each particle moving from one cell to the other and/or collected in a fiber cell by adhesion. Such a change in the system configuration was driven by the energy difference after and before the change, subject to random fluctuation captured by the Monte Carlo simulation. Simulations were carried out for the filtration process of particles of different sizes through fibrous filters with various fiber volume fractions. The simulation results were in good agreement with reported experiments, indicating validity of the approach.

Several advantages of the approach were demonstrated. With the use of a simple binary algorithm, this approach was capable of realistically simulating such complicated mechanisms as diffusion, interception and gravity effect involved in the filtration process. Also, it could be applied to explain various effects due to interactions at interfaces within heterogeneous materials.

Future work may include taking into account the movement of fiber substrate during filtration process, and modification of the model for the purpose of depicting more complex filtration processes involving poly-disperse particles and multi-layer filters.

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