Numerical investigation of aerosol deposition on a single 2D fiber

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The aerosol filtration technique deserves extensive attention, due to its wide applications found in health, environment, and industry. The simulation of aerosol filtration over fibrous filters involves the numerical investigation of the motion and capture of particles (aerosols) under different fluid operating conditions.

The capture of aerosol in fibrous filters involves the following deposition mechanisms: Impaction, interception, diffusion and gravitation. The motion of the particles is governed by the relevant forces acting on the particles. Due to the dilute concentration of the aerosol, the influence of particle motion onto the fluid and particle-particle interaction can be neglected. The particles are removed by a fibrous filter when they collide and stick to the surface of the fiber. An Euler-Lagrangian approach is engaged to simulate the particle trajectories. The air flow field (continuous phase) is simulated in Ansys CFX (Euler approach) and the particle trajectories (dispersed phase) are computed by Lagrangian simulations in MATLAB.

Real fibrous filters consist of a large number of fibers of non-uniform size and random orientation and position. For simplification, a single 2D fiber is considered and placed normal to the airflow to analyse several deposition mechanisms. The efficiency at which the particles are collected by a single fiber from an aerosol stream is called single-fiber efficiency \(E_{\Sigma}\), which is highly dependent on particle size. The particle motion is also affected by diffusion, where the dispersion of particles due to Brownian motion follows a Gaussian distribution. The diffusion coefficient can be inferred from the mean distance travelled by the particle and agrees well with the theoretical diffusion coefficient calculated from the Stokes-Einstein equation. The diffusion mechanism becomes significant at particle sizes below 0.2 \(\mu\)m. The single-fiber efficiency is determined considering all deposition mechanisms and compared with existing theoretical models.

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1 Capture efficiency

Fibrous filters are often characterized by their pressure drop and their capture efficiency. To have a consistent idea of the capture efficiency, researchers often use the concept of single fibre efficiency 

\[
E = \frac{(N_{\text{in}} - N_{\text{out}})/N_{\text{in}}}{N_{\text{in}}}
\]

where \(N_{\text{in}}\) is the number of incident particles on the projected area of a single 2D fibre and \(N_{\text{out}}\) the number of particles leaving without getting captured by the fibre.

The main mechanisms of particle deposition on fibers are interception, inertial impaction, diffusion, and gravitational settling, assuming that neither the particle nor the fibers are electrically charged and thus neglecting the effect of electrostatic attraction onto particle deposition. Deposition by interception occurs for particles that follow gas streamlines when they reach a distance smaller than the particle radius from the surface of the fiber. Inertial impaction occurs when the inertial forces of the particle are dominant and, therefore, the particle can no longer follow the streamline. Diffusion caused by Brownian molecular motion provides an increased probability of deposition, because the particle can strike the fiber by the irregular movement from a non-intercepting streamline.

To determine the net filter efficiency \(E\) two approaches can be used. The first and more accurate approach is the penetration approach shown in equation (1). It is valid as long as each individual efficiency acts independently and is less than 1. It is basically the product of the penetration due to the different mechanisms shown in equation (1). The alternative efficiency approach is estimating the filter efficiency from the addition of single-fiber efficiency through each deposition mechanism. This, however, may overestimate the efficiency due to collection of the same particle by different mechanisms, i.e. the capture of the particle could be counted twice [1].

\[
E_{\Sigma} = 1 - (1 - E_R)(1 - E_I)(1 - E_D)(1 - E_{DR})(1 - E_G)
\]

(1)

2 Modelling and implementation

Since the particle concentration is well below a volume fraction of \(10^{-4}\) it can be safely assumed that the particle movement does hardly affect the bulk fluid motion. This assumption leads to a decoupling of the fluid flow calculation from the particle tracking. The fluid flow is scaled with the fibre diameter \(d_f\) and inlet fluid velocity \(u_0\), and simulated with Ansys CFX using an Eulerian method. The 2D fibre, with scaled fibre diameter \(d_f^* = 1\), is simulated using a fictitious domain model [2], using a cubic domain (which is dependent on solidity \(\alpha\)) with an inlet area with uniform scaled velocity of \(u_0^* = 1\), an outlet with a uniform pressure and symmetry planes as the other walls. The computed flow field is then imported to MATLAB to track the particle trajectory using an in-house MATLAB algorithm, where the particle transport is described by the second Newtonian axiom, which calculates the particle acceleration vector \(\frac{du_p}{dt}\) at each time step. Based on time and acceleration, the
particle position \( x_p(t) \) can be determined by integration. The particle rotation differential equation is also considered if the particle rotation has an effect onto the particle movement. Hence, we engage

\[
\frac{dx_p}{dt} = u_p, \quad m_p \frac{du_p}{dt} = \sum F_i, \quad I_p \frac{d\omega_p}{dt} = T.
\] (2)

Here, \( m_p \) is the mass of the particle, \( I_p \) is the torque of inertia of the particle, \( \omega_p \) is the angular velocity of the particle, and \( T \) is the torque acting on the particle. For the net force acting on the particle \( F \), the following forces are considered: drag force, inertial force, pressure force from pressure gradient and buoyancy, added mass force, Saffman force, Magnus force, and diffusion force. The implementation of the scaled diffusion force into the Lagrangian formulation is unique to this work, to the extent that the Brownian force is implemented as

\[
F_d = G \sqrt{\left(\frac{\pi S_0}{\Delta t}\right)}
\]

(3). Here, \( G \) is a vector whose components are independent zero-mean, unit variance Gaussian random numbers and \( S_0 = \frac{2}{\pi S_c S_l^2} \) (\( S_c = \nu/D \) is the Schmidt number and \( S_l = t_0 u_0 / d_0 \) is the Stokes number, where \( t_0 \) is the particle relaxation time). The time scale \( \Delta t \) was freely chosen until now but in this work it was taken in the range of mean free time which is the average time between collisions of gas molecules. The diffusion mechanism can be validated by observing the particle movement due to diffusion in a stagnant fluid and calculating the diffusion coefficient and comparing it to theoretical values.

3 Results

The MATLAB algorithm is run for various combinations of particle diameter \( d_0 \), fluid velocity \( u_0 \), and solidity \( \alpha \) and compared with existing experimental results and theoretical models. It can be seen in fig.1 that the net capture efficiency \( E_{\Sigma} \) predicted by the algorithm, plotted against the scaled particle diameter, also referred to as the diameter ratio \( (R) \), follows the experimental results closely. At the lowest \( E_{\Sigma} \), the values diverge considerably, which can be explained by the number of particles present within the simulation. Due to computational restrictions, a total of 1000 particles is simulated, which appears to be not sufficient to give statistically-valid results in the range \( E_{\Sigma} < 0.01 \). This could be overcome by simulating more particles.

![Simulation parameter:](image)

- \( d_0 = 11 \mu m \)
- \( \alpha = 0.0434 \)
- \( u_0 = 0.3 \ m/s \)
- \( \rho_p = 985 \ kg/m^3 \)
- Fluid=Air under standard conditions

Fig. 1: Comparison of theoretical single-fiber efficiency calculated according to Stechkina [4] and Lee and Liu [5] for the experiments carried by Lee and Liu with the results from the current MATLAB simulations.

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