

A STUDY OF PARTICLE FLOW AND DEPOSITION IN FILTER MEDIA USING CFD

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ABSTRACT – Recently, nanoparticles have been largely employed in intelligent materials and human health. This creates a need for industrial nanoparticle filtration. In this preliminary study the air flow and particle deposition in a two-dimensional model filter media was studied. A statistical model was used to determine the location of the fibers and the commercial packages ANSYS Fluent[®] were used for the simulations. The conditions of no slip and free slip at the fiber surfaces were tested, showing a pressure drop of 64 Pa for the first and 43 Pa for second case, respectively. The results showed that the second situation agreed better with experimental data (42 Pa). Thereby, this condition was used to obtain the deposition of 0.5 μm particles, in which Eulerian-Lagrangian approach was used to represent the fluid and dispersed phases, respectively. It was observed a 45% particle deposition efficiency.

1. INTRODUCTION

The gas filtration aims the removal of solids from a gas stream and is an operation largely used in industrial process and also in edifications where the people live or work. According to the World Health Organization (WHO), airborne particles can cause many respiratory diseases and lead to a high level of death. The nanoparticles are even more harmful to the human health, since they are capable to reach alveolar regions. Beyond the concern with the human health, some industrial plants, such as pharmaceutical and semiconductor factories, require that the air inside the room is totally free of airborne particles and, thus, need to use many high efficiency filters.

The mathematical modeling of air and particle flow can help the understanding of the capture of solid materials by the filter media fibers. However, in filtration process the free path available to the flow of the gas is of the same order of magnitude of their molecules, and the gas sometimes cannot be treated as fluid. A parameter that can be used to define this limit is the Knudsen number, which represents the relation between the mean free path of fluid molecules and the characteristic length scale of the geometry. According to Zhou et al. (2013), when this number is less than 0.01, continuum flow is fully established and the Navier-Stokes (N-S) equations with no-slip boundary equations can be applied for fluid-wall interactions. For $0.01 < \text{Kn} < 0.1$, the N-S still can be used, however, the free-slip boundary condition for fluid-wall interactions is not valid and a partial slip should be applied. Above

$Kn = 0.1$ the flow begins to fail to be considered continuous and the flow behavior is described accurately by certain low-level methods solving the Boltzmann equation, e.g. direct Monte Carlo simulations (DSMC).

The filter medium used in this study presents values of Knudsen number varying from 0.008 to 0.20, with an average value of 0.05. In this case, the air can be treated as fluid for the most of the domain and a partial slip condition should be applied for fluid-wall interactions. As initial study, this work brings results using the minimum and maximum slip condition, which were compared to experimental data. A partial slip condition will be implemented in further studies.

2. METHOD

2.1 Model Construction

A simplified 2-dimensional computational domain for CFD simulation was constructed from a simulated fiber diameters distribution based on experimental study of filter medium samples and its statistical description. A probability density function fitted to the data obtained by analysis of scan electronic microscopy (SEM) images from these samples allowed the simulation of a new set of diameters to compose the simplified 2D domain. The log-normal, normal and beta distributions were tested along the data by the maximum-likelihood method. The former has provided the best fit to the experimental distribution, with a long tail toward larger diameters values. With the fitted statistical model and its descriptive statistics (geometric average - μ_g and geometric standard deviation - σ_g), a simulated set of fiber diameters was generated through Monte-Carlo simulation, given solid fraction in the studied filter medium and the dimensions of computational domain required. The tool used implements a truncated log-normal model that prevents the simulation of larger (and smaller) than observed diameters.

The size of computational domain was chosen in such way it accommodates at least 100 fibers. As stated by Zhou (2009), it is a requirement to the simplified 2D domain be statistically representative of the whole filter medium. The geometry has been constructed automatically by a script and the software ANSYS 14.5 Design Modeler®. Figure 1 shows the generated geometry and its dimensions. A 30 μm space was added to upstream and downstream regions to assure a smooth flow transition between bulk and the filter medium.

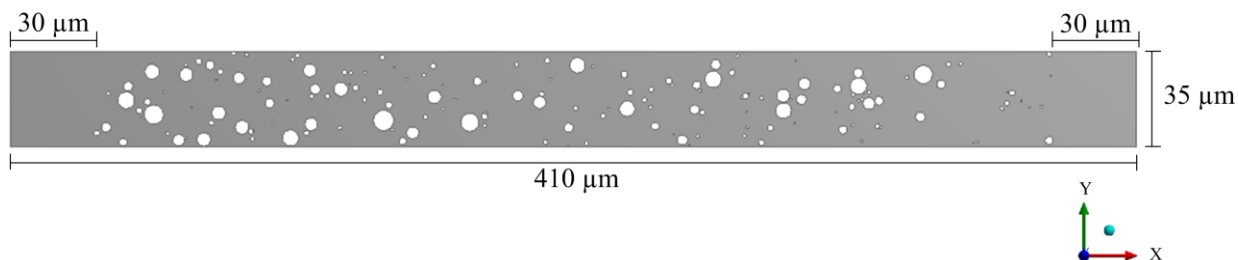


Figure 1 - Filter media and its dimensions.

2.2 Mesh Generation

To discretize the domain in finite volumes where the governing equations were solved, the software ANSYS 14.5 Meshing[®] was used. In order to verify the grid influence over the simulation, tetrahedral meshes with different levels of refinement were created. The pressure drop was monitored for three meshes with tetrahedral elements, with 42761, 46195 and 66456 control volumes. Since this test showed that the pressure drop remained almost constant for the three situations, the coarser mesh was used to the simulations and it is showed in Figure 2.

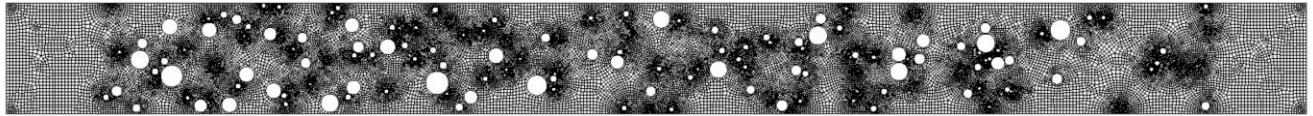


Figure 2 - Finite volume mesh.

2.3 Governing Equations

The continuity equation (Equation 1) and the momentum conservation equation (Equation 2) were solved for laminar and isothermal flow, at 298.15 K. The gravity is not included in the following governing equations since the filter medium can operate at any direction:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \bar{v}) = 0 \quad (1)$$

$$\frac{\partial (\rho \bar{v})}{\partial t} + \nabla \cdot (\rho \bar{v} \bar{v}) = - \nabla p + \nabla \cdot (\bar{\tau}) \quad (2)$$

where ρ is the air density (1.1842 kg m^{-3}), t is the time, \bar{v} is the fluid velocity vector, p is the pressure, \bar{g} is the gravity vector and $\bar{\tau}$ is the stress tensor, given by Equation (3):

$$\bar{\tau} = \mu \left[(\nabla \bar{v} + \nabla \bar{v}^T) - \frac{2}{3} \nabla \cdot \bar{v} I \right] \quad (3)$$

where μ is the air viscosity ($1.8446 \times 10^{-5} \text{ Pa s}$) and I is the unit tensor.

Since few particles were injected into the computational domain, the one-way coupling was used to represent the interaction between continuous and dispersed phases. This method considers that the solid phase has no influence on the fluid phase. The trajectory of the particles was predicted applying a force balance on each particle, using the Lagrangian reference frame, considering drag force and Brownian motion, as represented in Equation (4). In Lagrangian approach, the discrete phase is considered as points and the trajectory can be estimated for each particle individually.

$$\frac{d^2x_p}{dt^2} = \frac{18\mu}{\rho_p d_p^2} \frac{C_D Re_p}{24} (\bar{v} - \bar{v}_p) + \zeta_i \sqrt{\frac{\pi}{\Delta t} \frac{216\nu k_B T}{\pi^2 \rho \left(\frac{\rho_p}{\rho}\right)^2 C_C}} \quad (4)$$

where x_p , d_p , ρ_p , v_p and Re_p are the position, the diameter, the density (912 kg m^{-3}), the velocity vector and the Reynolds number of the particle, respectively, ζ_i are zero-mean, unit-variance-independent Gaussian random numbers, ν is the kinematic viscosity of the fluid, k_B is the Boltzmann constant, T is the absolute temperature, Δt is the time step, C_C is the Cunningham correction factor and C_D is the drag coefficient given by:

$$C_D = a_1 + \frac{a_2}{Re_p} + \frac{a_3}{Re_p^2} \quad (5)$$

where a_1 , a_2 e a_3 are constants given by Morsi and Alexander (1972) and Re_p is given by:

$$Re_p = \frac{\rho |\bar{v} - \bar{v}_p| d_p}{\mu} \quad (6)$$

The Cunningham correction factor was calculated by following equation, based on experimental data and largely used to estimate this factor, proposed by Davies (1945):

$$C_C = 1 + Kn \left[2.514 + 0.8 \exp\left(-\frac{0.55}{Kn}\right) \right] \quad (7)$$

where Kn is the Knudsen number, given by the ratio between mean free path of the gas molecules and the particle diameter.

2.4 Boundary Condition and Numerical Method

A constant velocity of 0.0617 m s^{-1} was used at the inlet of the domain and at the outlet a uniform pressure was considered. At the superior and inferior portions of the domain, named as walls in Figure 3, a free slip condition was applied. A symmetry condition was used at the filter media surfaces to represent the continuation of the filter. For the fibers surfaces, it was tested the no slip and free slip conditions and the results were compared to experimental results. The first one considers that the fluid assumes the same velocity as the surface, i.e. zero velocity, while in the free slip condition all the wall shear stresses are set to zero. For the particles, it was considered that they stay trapped when they collide with the fibers surfaces and with the walls shown in Figure 3.

For fluid and particles flow calculations, a fixed time step of $1 \times 10^{-5} \text{ s}$ was used. For advancing in time, the convergence criterion was that the RMS residuals were less than 10^{-5} . It was simulated 0.2 seconds and, at every time step, three particles with $0.5 \text{ }\mu\text{m}$ diameter were released at the domain entrance equally spaced. The total number of particles that entered in the domain at the end of the simulation was 60000.

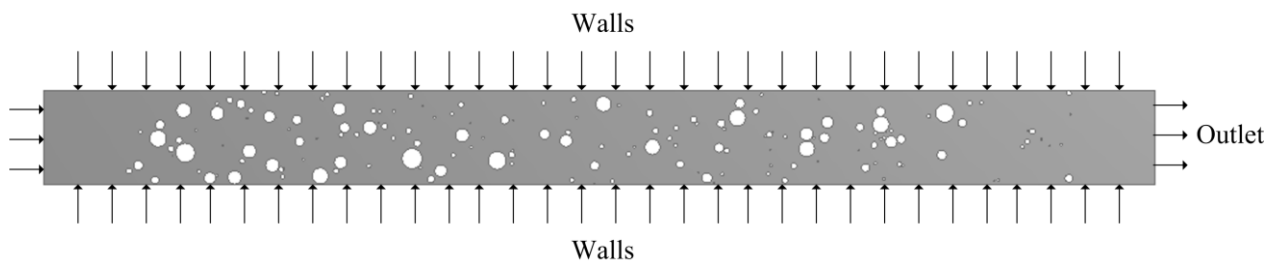


Figure 3 - Boundary conditions of the simulation.

The commercial code ANSYS 14.5 Fluent® was employed to run the calculations. The software applies the finite volume method for numerical solution of partial differential equations. In this method, the space is discretized in a finite number of control volumes, where the variables are calculated. The pressure-based approach was used in this study and it involves the manipulation of continuity and momentum conservation equations to obtain an equation to the pressure and, thus, determine the pressure and velocity fields. Furthermore, the pressures and diffusion gradients were approximated using the least squares cell based method and, to discretize the convective terms, the second order upwind difference scheme was applied. The transient terms were approximated by the first order implicit formulation. Finally, the segregate algorithm SIMPLE (Semi Implicit Linked Equations), that involves the resolution of the governing equations sequentially, was employed to solve the system of algebraic approximated equations. All the calculations were carried out considering double precision.

3. RESULTS

The pressure and velocity fields of the gas are shown in Figures 4 and 5 for free slip and no slip fluid-fibers interaction conditions, respectively. The velocity fields show some similarity, but it can be observed a bigger portion of the fluid around the fibers in the case that no slip condition with lower velocity, which was expected, since the fibers surfaces are stationary. The pressure fields are similar for the two cases, but the pressure drop for the first situation is about 43 Pa and, for the second one, the pressure drops is approximately 64 Pa. Tronville (2006) presented a pressure drop of 42 Pa for the same filter considered in the numerical study presented in this work. For the situation considering free slip, the pressure drop originates due a suddenly change in the geometry. The distributed fibers along the filter medium forces the fluid to change the path and this causes an energy loss that could be significant when the length of the fluid path is small, as the case of the filter medium. Therefore, it can be inferred that the free slip shows better agreement with experimental data than the no slip condition. In some cases, the gas molecules that collide with the fibers surfaces not reach the momentum equilibrium and the gas velocity adjust partially to the surface velocity, that is zero in most situations of fibers of filter media. In fact, the conditions of partial and complete slip are more realistic for all real gases. For these reasons, to evaluate the particle deposition efficiency of the filter media the free slip was used.

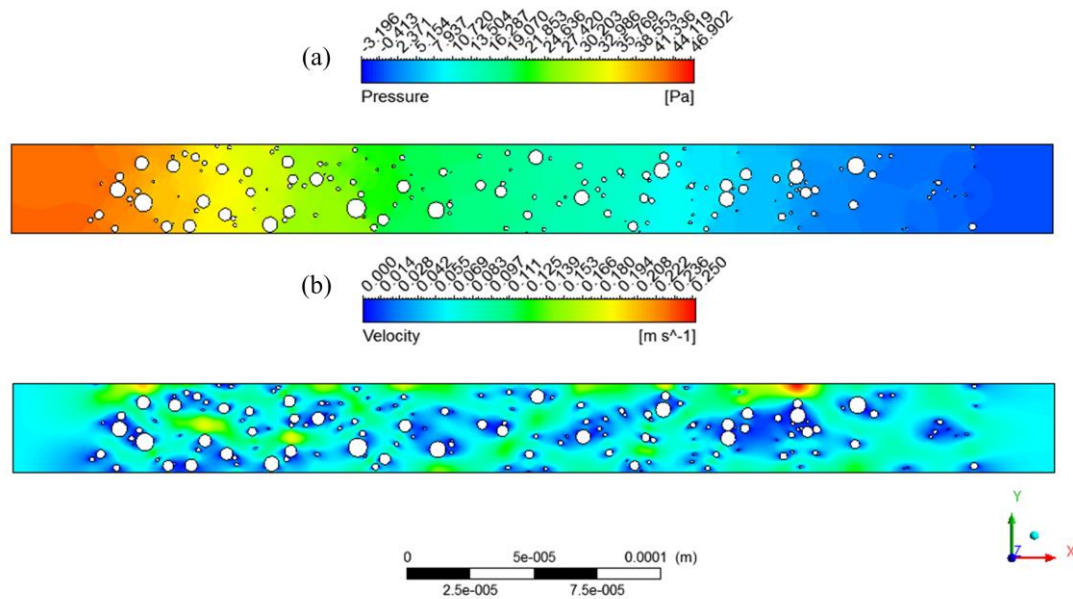


Figure 4 – Pressure (a) and velocity (b) fields for free slip condition on the fibers.

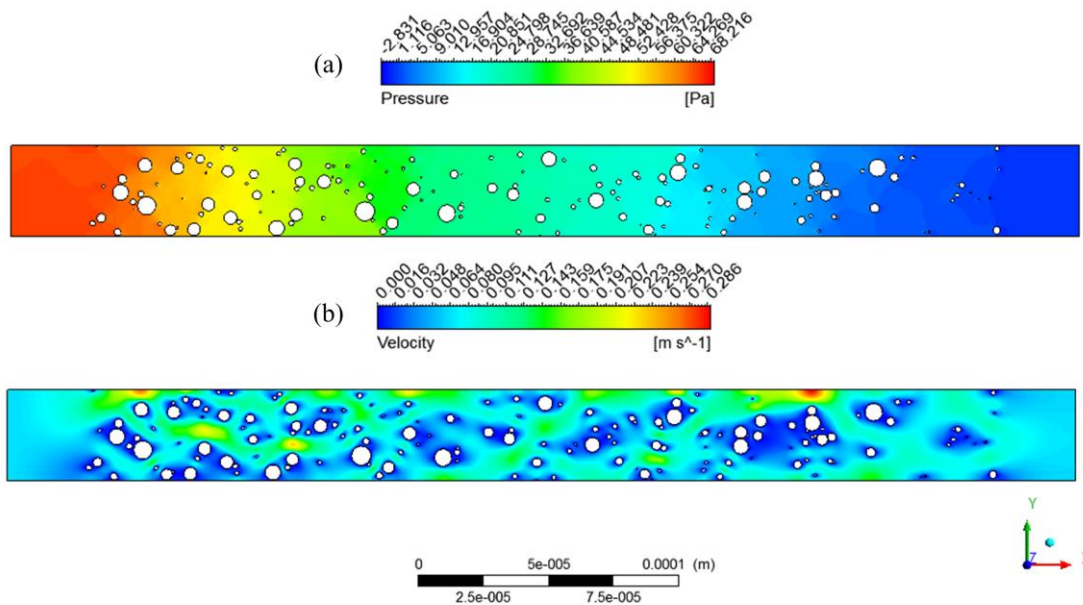


Figure 5 – Pressure (a) and velocity (b) fields for no slip condition on the fibers.

The numerical results showed a particle deposition efficiency of the filter media was 45%. The capture efficiency was calculated by the ratio of the deposited particles to those that entered in the computational domain. In Figure 6, it can be observed that most particles follow the fluid streamlines and leave the computational domain. No experimental data were obtained for this filter until this moment and, hence, no comparison can be made between simulated and experimental results.

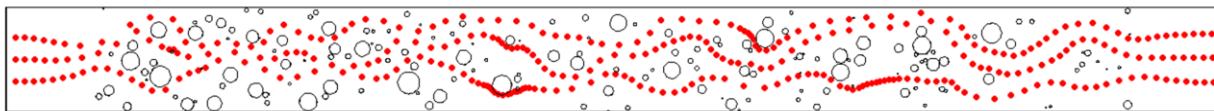


Figure 6 - Particle trajectory along the filter media.

4. CONCLUSIONS

The pressure and velocity fields and the particle deposition were studied in this work for a filter media with random fibers diameters localized according to a statistical model, in a two-dimensional computational domain. The free slip condition for the fluid on the fibers surfaces agreed better with experimental data than the situation considering no slip, showing a pressure drop of 43 Pa and 64 Pa, respectively. Besides, a particle deposition efficiency of 45% was observed. This study is still preliminary and many adjusts need to be implemented. For example, an expression for estimate the partial slip on the fibers surfaces, as proposed by Maxwell, and a random function to determine the injection points at the filter media inlet will be tested in next steps of the research.

5. REFERENCES

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